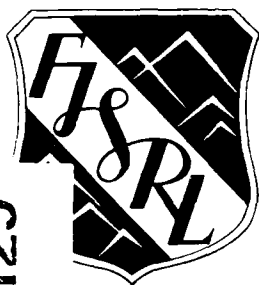# FJSRL-TR-89-0005

FRANK J. SEILER RESEARCH LABORATORY

NS(B) SPECTRUM

THEORY AND CODE

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CAPT R.I. LAWCONNELL

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AIR FORCE SYSTEMS COMMAND

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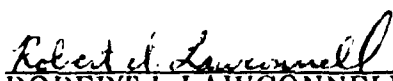
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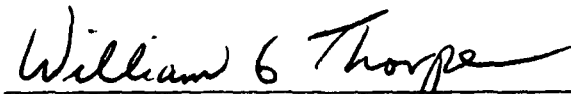
This technical report has been reviewed and is approved for publication.

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As part of an on-going effort to determine the rotational and vibrational population of the NS(B) molecule in an $S+N_3$ -- $NS(B) + N_2(X)$ reaction a spectrum code was written. This document outlines the basic theory used in writing the code, explains how to run the code along with providing a listing of the spectrum code and accompnaying files. It should be noted that even though this code was written specifically for the $NS(B^2\pi) - NS(X^2\pi)$ transition, it is easily modified to do a variety of other molecules and transitions.

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I.   INTRODUCTION

During the past year the Laser Kinetics Branch has been studying the $B^2\Pi - X^2\Pi$ transition in nitrogen–sulfide. We have been particularly interested in this transition because we think the B states 1μ second lifetime and large Franck–Condon shift make it a good short wavelength chemical laser candidate. As part of our study we have determined the rotational and vibrational populations of the excited molecule produced in an $S+N_3 \rightarrow NS(B) + N_2$ reaction. To do this accurately it was necessary to write a spectrum code. This document outlines the theory, explains how to run, and provides a listing of the spectrum code and accompanying files. It should be noted that even though this code was written specifically for the $NS(B^2\Pi) - NS(X^2\Pi)$ transition, it is easily modified to do a variety of other molecules and transitions.

II.   NS SPECTRUM CODE THEORY

The code is based on the quantum mechanics of Schrödinger. In the next few pages, I'll outline the most significant relations leading up to the electronic–ro–vibrational intensity relation which gives the intensity of a spectrum line as a function of wavelength.

The perturbed Schrödinger equation is given by.

$$\sum_k \frac{1}{m_k} \left[\frac{\partial^2 \chi}{\partial X_k^2} + \frac{\partial^2 \chi}{\partial Y_k^2} + \frac{\partial^2 \chi}{\partial Z_k^2} \right] + \frac{8\pi^2}{h^2} (E-V)\chi + \omega\chi = 0 \tag{2.1}$$

where m_k is the mass of the kth particle, χ is the wave function; X_k, Y_k, Z_k are the coordinates of the kth particle, E is the total energy, V is the potential energy, and $\omega\chi$ is the perturbing term. The interaction of an electromagnetic wave (with an electric vector $\vec{E}$) with an atomic system can be approximated as the interaction of $\vec{E}$ with the dipole moment ($\vec{M}$) of the atomic system. This interaction enters into Equation 2.1 as $\omega = \vec{E}\cdot\vec{M}$, where $\vec{M}$ has components $M_x=\Sigma e_k X_k$, $M_y=\Sigma e_k Y_k$, $M_z=\Sigma e_k Z_k$, and e_k is the change on the kth particle.

In solving the Schrödinger equation for an electromagnetically disturbed atomic system, Pauling and Wilson[1] found that if the system was originally in a state of energy,

E_n, there is a non-zero probability of finding it in a state of energy, E_m, if the emission of a photon of energy $hc\nu_{nm} = E_n - E_m$ is allowed. Specifically, the probability of a transition between two states n and m is proportional to the square of the matrix elements of the electric dipole moment ($\vec{R}^{nm}$).

The components of $\vec{R}^{nm}$ are defined as follows:

$$R_x{}^{nm} = \int \chi_n{}^*M_x\chi_m d\tau, \tag{2.2}$$

$$R_y{}^{nm} = \int \chi_n{}^*M_y\chi_m d\tau, \tag{2.3}$$

$$R_z{}^{nm} = \int \chi_n{}^*M_z\chi_m d\tau, \tag{2.4}$$

where χ_n, χ_m are the eigenfunctions of the two states, and the integral is over the total configuration space.[2]

The intensity of a spectral line for a transition from state χ_n to χ_m is given by:

$$I_{em}{}^{nm} = N_n hc\nu_{nm}A_{nm}, \tag{2.5}$$

where N_n is the number of atoms or molecules in the initial state, $hc\nu_{nm} = E_n - E_m = $ energy emitted in transition, A_{nm} is the Einstein transition probability of spontaneous emission and according to wave mechanics is related to the matrix elements of the electric dipole moment (as was previously shown for stimulated emission) as follows:

$$A_{nm} = \frac{64\pi^4\nu_{nm}{}^3}{3h}|\vec{R}^{nm}|^2 \text{ for non-degenerate levels.}$$

$$A_{nm} = \frac{64\pi^4\nu_{nm}{}^3}{3h}\frac{\Sigma|\vec{R}^n{}_i{}^m{}_k|^2}{d_p} \text{ for levels that are } d_p \text{ fold degenerate.} \tag{2.6}$$

Combining Equations (2.5) and (2.6) gives the intensity of the spectrum line in emission as:

$$I_{em}{}^{nm} = \frac{64\pi^4 \, hc\nu_{nm}{}^4}{3h}\frac{\Sigma|\vec{R}^n{}_i{}^m{}_k|^2}{d_p} \tag{2.7}$$

However, our experimental detectors only count the number of photons in a given frequency range. The number of counts at a given frequency can be obtained by dividing

Equation (2.7) by the energy associated with each photon at that frequency. Doing this yields the photon count as a function of frequency:

$$I_{emc}{}^{nm} = \frac{64\pi^4}{3h} N_n \, \nu_{nm}{}^3 \frac{\Sigma |\vec{R}^n{}_i{}^m{}_k|^2}{d_\rho} \tag{2.8}$$

The number of molecules, N_n, in the initial state depend on the electronic, vibrational, and rotational levels available, as well as the energy required to populate each level. In the following, we will determine the energy required to populate a given electronic–ro–vibrational state as well as the levels available. For equilibrium systems we know these states to be populated according to a Boltzmann distribution. This gives the number of molecules in each state once we know the total energy available to the system.

II.1. DETERMINATION OF ENERGY LEVELS

We know that the energy of a molecule is due to the motion of the electrons about the nuclei (electronic energy), vibration of the nuclei (vibrational energy), and rotation of the nuclei about the center of mass (rotational energy). We first will consider the rotational energy. If we approximate the molecule as a rigid rotator and substitute $m = \mu = \frac{M_1 M_2}{M_1 + M_2}$ and $V = 0$ into the Shrödinger equation (Equation 2.1), we obtain a solution for the rotational energy levels:

$$E_J = \frac{h^2 J(J+1)}{8\pi^2 I}, \tag{2.9}$$

where M_1, M_2 are the nuclear masses, and I is the moment of inertia of the rotator; J refers to the rotational level in question.

Now in spectroscopy it is customary and convenient to write all energies in terms of wave numbers. The wave number is obtained by dividing the energy by hc. So, in wave numbers Equation (2.9) becomes

$$\frac{E_J}{hc} = F(J) = \frac{hJ(J+1)}{8\pi^2 c I} = B\,J(J+1) \text{ (cm}^{-1}) \tag{2.10}$$

$B = \frac{h}{8\pi^2 c I}$ is called the rotational constant. The wave number (or energy) associated with a transition from one rotational level to another is:

$$\nu = F('') - F(J''), \tag{2.11}$$

where J' *always refers to the* upper rotational level and J'' refers to the lower.

It is well known that molecules not only rotate about their center of mass, the nuclei vibrate with respect to one another. For a diatomic molecule, the molecule vibrates along an imaginary line joining them and passing through their respective centers. The coulombic force holding the nuclei together goes as $-kx$. The potential energy associated with this is $V = \frac{kx^2}{2}$ or that of a harmonic oscillator. If one substitutes this into the Schrödinger equation and solves for the energies of the vibrational levels, the following wave numbers (or energies) are obtained:

$$\frac{E(v)}{hc} = G(v) = \omega\,(v + \tfrac{1}{2}), \tag{2.12}$$

where ω refers to the fundamental frequency of vibration between the nuclei, and v corresponds to the allowed vibrational levels. The wave number associated with a transition from one vibrational level to another is:

$$\nu = G(v') - G(v''), \tag{2.13}$$

where v' refers to the upper vibrational level and v'' refers to the lower level.

Of course the sum of potential energy of the nuclei and the electronic energy of the electrons forms the potential well in which the nuclei carry out their vibrations. It turns out that this potential well is harmonic to first order (very small amplitude vibrations about the equilibrium displacement between the nuclei) but is anharmonic if larger displacements from equilibrium are considered. This anharmonic effect can be taken into account by using a potential of the form (instead of $V = \frac{kx^2}{2}$):

$$v = \frac{kx^2}{2} - gx^3, \tag{2.14}$$

where $x = r - r_e$, r_e is the equilibrium separation of the nuclei, and g is much smaller than $k/2$. If this potential is substituted into the Schödinger equation, the following anharmonic–oscillator wave numbers (energies) are obtained:

$$\frac{E_v}{hc} = G(v) = \omega_e(v+1/2) - \omega_e x_e(v+1/2)^2 + \omega_e Y_e(v+1/2)^3 + \dots \tag{2.15}$$

Previously, we considered the rotational energies of a molecule on the basis of it being a rigid rotator. It is quite obvious that if the molecule is vibrating it is not rigid. In a rather involved wave mechanical calculation, Pauling and Wilson[1] show that if one takes into account the molecular vibrations or rotations the following wave numbers for a given rotational (J) and vibrational (v) level are given:

$$F_v(J) = B_v J(J+1) - D_v J^2(J+1)^2 \tag{2.16}$$

where

$$B_v = B_e - \alpha_e(v+1/2), \tag{2.17}$$

$$D_v = D_e + \beta_e(v+1/2), \tag{2.18}$$

$$B_e = \frac{h}{8\pi^2 c I_e} \quad \text{(see Equation 2.10)}, \tag{2.19}$$

$$D_e = \frac{4B_e^3}{\omega_e^2}, \tag{2.20}$$

α_e and β_e are much smaller than B_e and D_e respectively.

Finally, we consider the electronic energy states associated with the electrons about the nuclei. This energy is obtained by considering the electrons interacting with each other and the nuclei. There is no exact solution of the Schödinger equation for these. One can estimate the energies of each level for a given molecule using the Born–Oppenheimer approximation.[3] However, in practice the electronic energies are observed spectroscopically and used to give the base energy of each electronic level. In terms of wave numbers this energy is given by:

$$T_e = T_0 + A\Lambda\Sigma, \tag{2.21}$$

where T_0 represents the energy of the electronic state (base energy) neglecting energy splitting of levels due to electron spin, A is the spin orbit coupling constant, Λ represents the component of electronic orbital angular momentum along the internuclear axis, and Σ is the sum of electron spins for the molecule.

If the electronic orbital angular momentum is given by a vector $\vec{L}$ with magnitude $L=|\vec{L}|$ then the allowed quantum numbers representing the component of electronic angular momentum along the internuclear axis are given by:

$$\Lambda = 0, 1, 2, ..., L \tag{2.22}$$

One should note that $\Lambda = 0, 1, 2, ...$ corresponds to the molecular state designation Σ, Π, Δ, ... (e.g., NS($B^2\Pi$) refers to nitrogen sulfide in a state with $\Lambda = 1$). T_0 in equation (2.21) above is also a function of Λ.

If the total electron spin associated with the molecule is $\vec{S}$ and the magnitude of, this spin is given by $S = |\vec{S}|$, then $\vec{S}$ will precess about the field direction (in this case the internuclear axis) with a constant component $\Sigma(h/2\pi)$. Quantum theory allows the following values of $\Sigma = S, S-1, ... -S$. \hfill (2.23)

The total number of Σ values for a given S from Equation (2.23) is given by:

$$M = 2S + 1, \tag{2.24}$$

where M is called the multiplicity of the state. The multiplet structure observed in electronic bands is due to the electron spin and the slightly different energy levels corresponding to the different electron spins given in Equation (2.23). The electronic energy of the multiplet is given by Equation (2.21). Note that if $\Lambda = 0$ for a Σ state, there can be no spin related splitting or multiplet structures. This is because when $\Lambda = 0$ there is zero orbital angular momentum of the electrons and therefore no axial magnetic field. Since this field causes the spin splitting there can be no splitting even if there is a non–zero multiplicity. So, a $^2\Sigma$ state has a multiplicity of M=2, but because $\Lambda=0$ there is no multiplet splitting.

The component of the total angular momentum of the electrons along the internuclear axis is given by:

$$\Omega = |\Lambda + \Sigma|. \tag{2.25}$$

This plus the quantum number for rotation (call it $\vec{N}$) of the nuclei gives the resultant total angular momentum $\vec{J}$. If the interaction of the electronic motion and the nuclear rotation is small, but the electronic motion is strongly coupled to the line joining the nuclei, Ω is well defined. This is typically referred to as a Hund's case a. There are a

variety of cases (see Hertzberg); however, for NS Hund's case a applies. So, combining all the energy (wave number) terms for a molecule we obtain the following sum:

$$\frac{E_{tot}}{hc} = T_e + G(V) + F(J) \tag{2.26}$$

The wave number associated with the emission of a photon or the transition from one state (n) to another (m) is given by:

$$\frac{h\nu'}{hc} = \nu_{nm} = T_e' - T_e'' + G(v') - G(v'') + F(J') - F(J'')$$

From Equations (2.15–2.20), this becomes:

$$\nu_{nm} = T_e' - T_e'' + \omega_e'(v'+1/2) - \omega_e'\chi_e'(v'+1/2)^2 - \omega_e''(v''+1/2) + \omega_e''\chi_e''(v''+1/2)^2 + \ldots$$
$$+ B_v'J(J'+1) - D_v'J'^2(J'+1)^2 - B_v''J''(J''+1) + D_v''J''^2(J''+1)^2 + \ldots. \tag{2.27}$$

This corresponds to the wave number of the emitted photon if the transition is allowed. Using quantum mechanics it is straightforward to show that molecular transitions from one particular state to another are generally allowed if:

$$\Delta J = J' - J'' = 0, \pm 1 \tag{2.28}$$

and for Hund's case a:

$$\Delta \Lambda = \Lambda' - \Lambda'' = 0, \pm 1 \tag{2.29}$$

$$\Delta \Sigma = \Sigma' - \Sigma'' = 0. \tag{2.30}$$

Note that $\Delta v = v' - v''$ is not restricted in any way.

So, if we apply this to the proposed $NS(B^2\Pi) - NS(X^2\Pi)$ transition, we first note that since the upper and lower states are $^2\Pi$'s, $\Lambda = 1$ for both and $\Delta\Lambda = 0$. Since $M = $ multiplicity $= 2S + 1 = 2 \Rightarrow S = 1/2$ or $\Sigma = \pm 1/2$. So, $\Omega = |\Lambda + \Sigma| = 1/2, 3/2$. However, since $\Delta\Sigma = 0$ in Hund's case a the possible electronic transitions are restricted to the following:

$$B^2\Pi_{1/2} - X^2\Pi_{1/2} \text{ and } B^2\Pi_{3/2} - X^2\Pi_{3/2},$$

where Ω has been written as the subscript on the Π (orbital angular momentum corresponding to $\Lambda = 1$).

Keeping in mind that $\Delta J = 0, \pm 1$ in Equation (2.27), one can represent the possible transitions for the $NS(B^2\Pi) - NS(X^2\Pi)$ graphically (see Fig. 1). R_1, Q_1, P_1 correspond to

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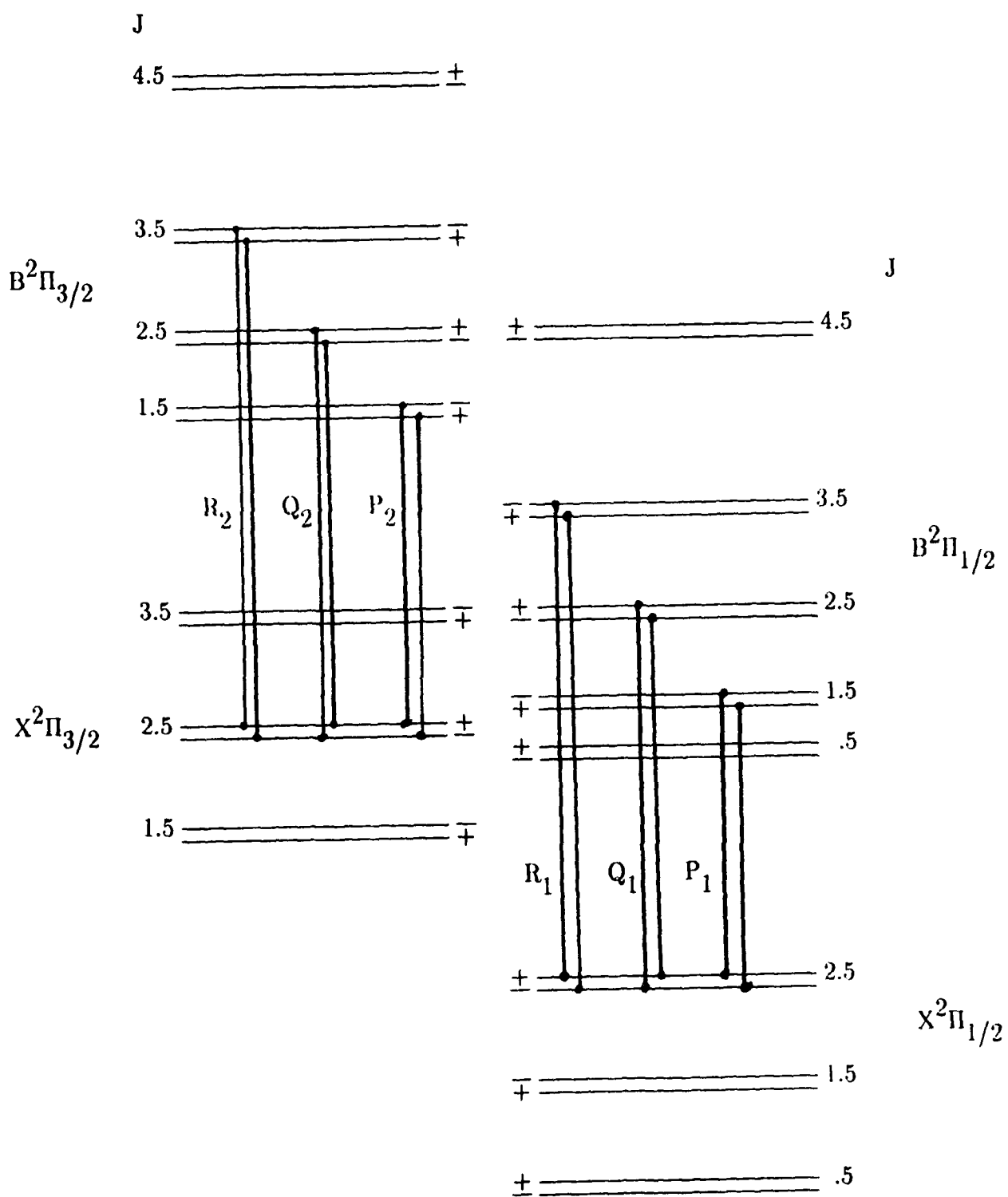
Figure 1. Energy Level Diagram for NS(B²Π)–NS(X²Π) Bands[2]

the branches with ΔJs of $+1, 0, -1$ respectively for the $^2\Pi_1/_2$-$^2\Pi_1/_2$ transitions. R_2, Q_2, P_2 correspond to ΔJs of $+1, 0, -1$ respectively for the $^2\Pi_3/_2$-$^2\Pi_3/_2$ transitions.

II.2. POPULATION OF ENERGY LEVELS

Up to this point we have considered the electronic, rotational and vibrational energy levels available to a molecule. We have also considered the allowed transitions from one state to another. Since we have determined the energy levels available we now need to figure how many molecules populate any given level. Often in nature, systems exist in states of thermal equilibrium. This is typically true of the molecules we study. For this reason we first consider obtaining the populations of electronic–ro–vibrational energy levels for molecules in thermal equilibrium.

Electronic Distribution Function

First, we consider the electronic distribution function for a doublet state in thermal equilibrium (we consider doublets because of the doublet NS transitions). For a doublet state in equilibrium the number of molecules in the upper electronic state with a given Ω is given by (we are interested in the upper state because we want to produce an emission spectrum) a Boltzmann distribution:

$$N_{E\Omega} = \frac{Ne^{-\epsilon_\Omega/kT_E}}{\Sigma e^{-\epsilon_\ell/kT_E}} \tag{2.31}$$

where ϵ_Ω is the energy in wave numbers of the different electronic levels associated with different values of Ω (with $\epsilon_{min} \equiv 0$). Min is the minimum Ω value and $k = .695$ cm^{-1}/°kelvin. For NS we have

$$N_{E_1/2} = \frac{Ne^{-\epsilon_1/2/kT_E}}{\Sigma e^{-\epsilon_\ell/kT_E}} = \frac{N}{e^{-\epsilon_1/2/kT_E} + e^{-\epsilon_3/2/kT_E}} \tag{2.32}$$

and with $\epsilon_{min} = \epsilon_1/2 = 0$, $\epsilon_3/2 = 90$, $kT_E = 200$ cm^{-1} at room temperature, where $T_E = 300$°k = the electronic temperature.

$$N_{E_{1/2}} = N(.61)$$

$$N_{E_{3/2}} = \frac{Ne^{-\epsilon_{3/2}/kT_E}}{\Sigma e^{-\epsilon_\ell/kT_E}} = N(.3893)$$

So, for NS in the B state the $\Omega = 1/2$ level has 5/3 the population of the $\Omega = 3/2$ level.

Vibrational Distribution Function

For vibrational levels in thermal equilibrium the population of the different energy levels is given very accurately by a Boltzmann distribution. The number of molecules in a given vibrational level is

$$N_v = \frac{N}{Q_v} e^{-G_0(v)hc/kT_v} \tag{2.33}$$

where $Q_v = 1 + e^{-G_0(1)hc/kT_v} + ...,$ \hfill (2.34)

$= $ state sum,

$$G_0(v) = G(v) - G(0), \tag{2.35}$$

$T_v = $ the vibrational temperature.

It should be noted that if we are concerned with emission, $G_0(v)$ and N_v correspond to the upper state. The $G(v)$ above is given by Equation (2.15).

Rotational Distribution Function

The number of molecules found in a given rotational energy level in thermal equilibrium is given by a Boltzmann distribution function times the degeneracy of the level which is usually $2J+1$. This is because, for a given energy each of $2J+1$ degenerate levels may be populated. The number of molecules in a given J level is given by:

$$N_J = \frac{N(2J+1)e^{-F(J)hc/kT_r}}{Q_r}, \tag{2.36}$$

where F(J) is given by Equation (2.16),

$$Q_r = 1 + 3e^{-F(1)hc/kT_r} + 5e^{-F(2)hc/kT_r} + ..., \tag{2.37}$$

$T_r = $ the rotational temperature.

Now F(J), to good approximation, can often be set equal to:

$$F(J) = B_v J(J+1).$$

If this is substituted into (2.36) and (2.37),

$$Q_r = 1 + 3e^{-2B_vhc/kT_r} + 5e^{-6B_vhc/kT_r} + \dots \tag{2.38}$$

$$\simeq \frac{kT_r}{hcB_v} \text{ for large } T_r \text{ and small } B_v, \text{ which is usually the case.} \tag{2.39}$$

T_r is usually greater than 300°K and B_v is about .6 for NS. This makes (2.39) a good approximation. This implies that

$$N_J \simeq \frac{NhcB_v}{kT_r}(2J+1)e^{-B_vJ(J+1)hc/kT_r}. \tag{2.40}$$

At this point we are in a position to fairly accurately define N_n of Equation (2.8) by using (2.31), (2.33) and (2.36):

$$N_n' \propto N_{E\Omega'}N_{v'}N_{J'}$$

$$N_n' = \frac{Ne^{-\epsilon_{\Omega'}/kT_e}}{\sum_\ell e^{-\epsilon_\ell/kT_e}} \cdot \frac{e^{-G_o(v')hc/kT_{v'}}}{Q_{v'}} \cdot \frac{B_{v'}}{T_r}(2J'+1)e^{-B_{v'}J'(J'+1)hc/kT_r} \tag{2.41}$$

n' of course corresponds to the upper state with Ω', J', v'.

II.3. ELECTRONIC–RO–VIBRATIONAL INTENSITY (COUNT) FUNCTION

We almost have everything we need to define Equation (2.8) for the NS molecule. N_n of (2.8) is given by Equation (2.41), ν_{nm} of (2.8) is given by (2.27). d_p of (2.8) is equal to the degeneracy of the levels which is $2J+1$. In the literature

$$\sum|\vec{R}^{n}{}_i{}^m{}_k|^2 \equiv |\vec{R}_{v'v''}|^2 S_{J'J''} \simeq \vec{R}_e{}^2 q_{v'v''} S_{J'J''}, \tag{2.42}$$

where the $R_{v'v''}$ is the part of the transition probability depending on the electronic and vibrational eigenfunctions and $S_{J'J''}$ is the part of the line strength that depends on J (the total angular momentum) and is called the Hönl–London factor.[4] In the following we will show how $\vec{R}_{v'v''} \simeq \vec{R}_e{}^2 q_{v'v''}$ and define all terms. The electronic and vibrational part of the eigenfunction can be written as:

$$\chi = \chi_e\chi_v. \tag{2.43}$$

The probability of a transition between two different (as shown in Equation (2.2–4)) electronic–vibrational states is given by:

$$|\vec{R}|^2 = |\int \chi'\vec{M}\chi d\tau|^2 \qquad (2.44)$$

The only parts of the electric moment $\vec{M}$ that can contribute to $\vec{R}$ are those that depend on the coordinates of the electrons. Rewriting (2.44) and substituting (2.43) with this in mind gives:

$$\vec{R} = \int \vec{M}e\ \chi_e'^*\chi_v'^*\chi_e''\chi_v''d\tau \qquad (2.45)$$
$$= \int \chi_e'^*\vec{M}_e\ \chi_e''d\tau_e \int \chi_v'^*\chi_v''d_r.$$

where χ_v' χ_v'' correspond to the vibrations of the nuclei along r and therefore only contribute along r, M_e and χ_e depend on the electronic coordinates only and contribute accordingly.

The first integral

$$\vec{R}_e = \int \chi_e'^*\vec{M}_e\chi_e''d\tau_e \quad , \qquad (2.46)$$

is called the electronic transition moment. This transition moment depends only slightly on the internuclear separation of the nuclei. For this reason $\vec{R}_e$ is often approximated by its average value over a transition:

$$\vec{R}_e \simeq \vec{R}e \qquad (2.47)*$$

The second integral of (2.45) is called the overlap integral. It basically states that a transition is more probable if the wave functions simultaneously have large values for the two vibrational states at a given internuclear separation. This embodies the Franck–Condon principle. As a result the overlap integral is often written in this way:

$$|\int \chi_v'^*\chi_v''dr|^2 = q_{v'v''}, \qquad (2.48)$$

where $q_{v'v''}$ is the Franck–Condon factor.

Note, sometimes one must include the variation $\vec{R}_e(\bar{r})$ with $\bar{r}$ to accurately model the spectrum. This happens to be the case for NS. As a function of the r–centroids ($\bar{r}_{v'v''}$) of the molecule Re is given by:[5]

$$Re = |\vec{R}e(\bar{r})| = Const.(-1+1.767\bar{r}_{v'v''} - 1.037\bar{r}^2_{v'v''} + .202\ \bar{r}^3_{v'v''}) \qquad (2.49)$$

where $\bar{r}_{v',v''}$ is the average separation of the nuclei for the v' to v'' transition.

Now, all the terms are defined necessary to give the intensity of a spectral line for an electronic–ro–vibrational transition from one state to another in equilibrium. Substituting (2.41, 42) into 2.8 we have:

$$
I_{J''v''\Omega}^{J'v''} = \frac{64\pi^4 N}{3h} \cdot \left[\overbrace{\frac{e^{-\epsilon\Omega/kT_E}}{\sum_\ell e^{-\epsilon\ell/kT_E}}}^{N_e \ \text{term}} \right] \cdot \left[\overbrace{\frac{e^{-G_0(v')hc/kT_{v'}}}{Q_{v'}}}^{N_v \ \text{term}} \right]
$$

$$
\cdot \left[\frac{\overbrace{B_v'e^{-B_v'J'(J'+1)hc/kT_r}}^{N_J \ \text{term}}}{T_r} \right]
$$

$$
\cdot \nu^3 Re^2 q_{v'v''} S_{J'J''} \tag{2.50}
$$

For NS, we first used Equation (2.50) to obtain the equilibrium synthetic spectrum at high pressures. The synthetic spectrum closely matched the experimental spectrum.

The low pressure cases (<2 Torr) had non–equilibrium rotational and vibrational distributions. We substituted our guesses for the distributions ($N_v + N_J$ terms in (2.50)) into the code until the synthetic spectrum matched the experimental spectrum. In this way we determined the non–equilibrium vibrational and rotational population distributions of the experimental spectrum. Such a comparison is shown in Figure 2, in which the relative populations of the vibrational levels $v' = 0$–6 (for $B^2\Pi_1/2 - X^2\Pi_1/2$ and $B^2\Pi_3/2 - X^2\Pi_3/2$ transitions) are given. The N_J term is given in *FUNCTION XI of the code*, run at a rotational temperature of 1400°K.

III. HOW TO RUN THE CODE

To run the NS($B^2\Pi$) – NS($X^2\Pi$) spectrum code one needs to first get in the directory where it resides. It is stored there along with files filled with Franck–Condon factors (FRANK.CON), Dunham coefficients (DUNHAM.COF), r–centroids (RCENTROID.DAT), the population weights (POPLTN.WT), file of data file names (FILE.OMA), and the experimental data files (named in FILE.OMA). These files must be present when running the program.

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First one must login to the VAX as follows:

    C   FJ

USER: LAWCONNELL

PASSWORD: ***   , see Captain Lawconnell.

Then default the directory to ASPECTRUM by typing:

    Sd.ASPECTRUM

Assuming all the Dunham coefficients, Franck–Condon factors, etc., mentioned above are available, all one need do is type:

    RUN SPNS

This activates the executable code found in file SPNS.EXE. The program is interactive and the input required is self–explanatory. The user will be asked to input the device on which to plot the spectrum, the spectrum title, the rotational and vibrational temperature, whether it is desired to plot experimental data versus the theory, etc. If one wishes to input non–equilibrium population weights for the upper state vibrational levels, this is done by modifying the file POPLTN.WT and specifying that a non–equilibrium distribution is required when asked while doing the input.

There is a file called INPUT.DAT that saves all the input parameters. If one is running a variety of cases that are similar this file will be accessed to give the input. The code prompts for any new changes. In addition the code produces three output files: 1) CHECK.OUT which contains the vibrational transition lines – and other information that indicates whether or not all is well with the run, 2) OUTPUT.SPEC which contains a list of intensities versus wavelength and 3) the plot file (as specified by the user).

Most features of the code are documented internally. The file structure for the various data files mentioned earlier can easily be determined by examining the respective read statements in the code. This also applies to the output files.

If one needs to transfer data from the OMA to the VAX one way to do it is to take a floppy of the data (DOS format) and use a PC along with KERMIT to transfer the data. The procedure for this is outlined below:

Type:

    %S

    KERMIT

    SERVER

Hit the <ALT> key

Type:

    K

    S   (to send)

    A:*.*

    .

    F   (to finish)

If the procedure failed start over by typing:

    <ALT>

    EXIT

    VAX

    EXIT

and then start with the KERMIT command and proceed as before.

Finally, if one needs to modify the code to do some problem of interest it is necessary to know how the previously presented equations relate to the code. If we start at the top, the first routine encountered is the program driver. In it are documented all the references used in writing the code and for producing the input files. The program driver is responsible for the program flow from plot driver initialization, through the spectrum generation, to the output of the spectrum.

The next routine is called SUBROUTINE INPUT. It reads in the experimentally derived Dunham coefficients. Dunham's equation combines Equations (2.15–21) into one equation:

$$T = \Sigma_{\ell j} \, Y_{\ell j}(v+1/2)^j \, J^j(J+1)^j \tag{2.51}$$

where the $Y_{\ell j}$ are the Dunham coefficients. From Equation (2.15–21) it is easily determined that the Dunham coefficients correspond to:

$$Y_{00} = T_e \qquad Y_{01} = B_e \qquad Y_{02} = -D_e \quad \ldots$$
$$Y_{10} = \omega_e \qquad Y_{11} = -\alpha_e \quad \ldots$$
$$Y_{20} = -\omega_e \chi_e \quad \ldots$$

These are the values found in the file DUNHAM.COF. We typically only use the values in the dashed box to model the NS spectra to the resolution of our spectrometer. It should be noted that there is a different group of Dunham coefficients for each electronic level – four groups for NS. This is referenced[6] and explained in greater detail within the code.

The Franck–Condon factors ($q_{v'v''}$) of Equations (2.48) and (2.50) are given in file FRANK.CON.[5] These are read in SUBROUTINE INPUT. In addition the $\bar{r}$–centroids[5] ($\bar{r}_{v'v''}$) of Equation (2.49) are also read.

If a non–equilibrium vibrational distribution is needed the N_v term of Equation (2.50) is replaced by the population weights found in file POPLN.WT. These are also read in INPUT. In addition the rotational temperature (T_r) and vibrational temperature (if equilibrium) are read in for the N_J and N_v terms of (2.50) respectively.

$G_0(v)$, Q_v, B_v, T_E, ϵ_Ω (Equations 2.15, 35; 2.34; 2.17; 2.32; 2.32 respectively) are obtained in SUBROUTINE INTENSE. These values are used there to calculate the N_E, N_v and N_J terms of Equation (2.50). All but the rotational part of Equation (2.27) is calculated in this routine and stored in matrix TRW.

The rotational part of (2.27), taking into account the P, Q, and R branching, is done in SUBROUTINE DOUBLET. This allows for the determination of the ν in equation (2.50). DOUBLET then calls SUBROUTINE AINT which gives the Hönl–London factors $(S_{J'J}'')$ of equation (2.50).

Since the final intensity is normalized, the actual value of N and the constants of equation (2.50) are not important. All the terms mentioned in (2.50) are brought together in FUNCTION XI. This is where the intensity of a given spectral line is calculated. These intensities are redistributed according to a Lorentzian slit width broadening redistribution function in SUBROUTINE LORNTZN:

$$I \cong I_0 \frac{\gamma^2}{(\lambda - 1 \times 10^8/\nu_{J'J''})^2 + \gamma^2}, \tag{2.52}$$

where $\gamma =$ the spectral resolution in Angstroms (which is on the order of two Angstroms for our OMA so that Doppler broadening was not considered),

$\lambda =$ the wavelength,

$1 \times 10^8/\nu_{J'J''} = \lambda_{J'J''} =$ the wavelength of the given transition one is redistributing.

$I_0 =$ original intensity of the line.

The experimental data is read in, spliced and weighted in SUBROUTINES LOADFIL, SPLICE and WEIGHT, respectively. The data and the synthetic spectra are normalized and plotted in SUBROUTINE OUTPUT (as specified by the user).

IV. NS(B – X) SPECTRUM CODE LISTING, FILES AND SAMPLE SPECTRUM

What has been written above is embodied and takes a functional form in the following program listing. In addition, the files used to run the code are also included (they follow the code). Finally, a sample spectrum (Fig. 2) comparing the code output to experiment is included. It should be noted that the theory and experiment correspond fairly well. This was true of all the spectra generated with the code and compared to experiment (for a variety of rotational temperatures and pressures).

```
C        PROGRAM SPECTRM
*****************************************************************
*
*           WRITTEN BY:
*
*                        CAPT BOB LAWCONNELL
*                        FRANK J. SEILER RESEARCH LABORATORY
*                        UNITED STATES AIR FORCE ACADEMY
*                        COLORADO SPRINGS, COLORADO  80840
*                        PHONE: 719-472-3502, AV 259-3502
*
*    THIS PROGRAM COMPUTES AND PLOTS THE NS(B) TO NS(X) SPECTRUM
*
*
*REFERENCES: 1) G. HERZBERG, SPECTRA OF DIATOMIC MOLECULES, VNR C 1950,
*               P.201,268-271.
*               - RELATION GIVING INTENSITY OF LINE FOR TRANSITION
*            2) M. BORN AND R. OPPENHEIMER, ANN PHYSIK 84,457(1927).
*               - BORN-OPPENHEIMER APPROXIMATION
*            3) OBASE,ET AL, J CHEM PHYS 89,257(1988).
*               - FRANCK-CONDON FACTORS, R CENTROIDS, ETC. FOR NS
*            4) J. JEFFRIES, ET AL, J PHYS CHEM, IN PRESS, 1 DEC 87
*               - EXPERIMENTALLY MEASURED TRANSITION PROBABILITIES
*                 (IE. RE**2).
*            5) R. ENGLEMAN JR.,ET AL, LA-4364,UC-34,TID-4500.
*               - AINT SUBROUTINE FOR HONL-LONDON FACTORS IN
*                 DOUBLET TO DOUBLET TRANSITIONS
*            6) I. KOVACS, ROTATIONAL STRUCTURE IN THE SPECTRA OF
*               DIATOMIC MOLECULES, AMER. ELSEVIER PUB, OUT OF PRINT,
*               1969.
*               - BASIS OF AINT SUBROUTINE
*            7) K. P. HUBER AND G. HERZBERG, MOLECULAR SPECTRA AND
*               MOLECULAR STRUCTURE, VOL IV, VNR C 1979, P486-487.
*               - DUNHAM COEFFICIENTS FOR NS
*
*****************************************************************
C
        PARAMETER(NROT=125)
C
C THE COMMONS ARE DIMENSIONED AS FOLLOWS (THEY MUST BE
C DIMENSIONED GREATER THAN OR EQUAL TO THE INDICATED
C VARIABLES):
C
C        COMMON/FACT/F(NF,20,20),Y(ND,ND1,2),G(ND,20),
C      1 B(ND,20),DG(ND,20)
C        COMMON/P    /TRB(6,20,20),P1(6,NROT),P2(6,NROT),
C      1 P1INT(6,NROT),P2INT(6,NROT)
C        COMMON/Q    /Q1(6,NROT),Q2(6,NROT),
C      1 Q1INT(6,NROT),Q2INT(6,NROT)
C        COMMON/R    /R1(6,NROT),R2(6,NROT),R1INT(6,NROT),
C      1 R2INT(6,NROT),FINT(6,10000),FIN(10000),FINX(10000)
C        COMMON/TEMP/TV,TR
C
C WHERE, NF=NT=THE NUMBER OF GROUPS OF FRANK-CONDON FACTORS --
C            1 GROUP PER ELECTRONIC TRANSITION,I.E. B3/2 TO X3/2
C            AND B1/2 TO X1/2 FOR NS.
C        NF1= V PRIME MAX INDEX (UPPER STATE)
C        NF2= V DOUBLE PRIME MAX INDEX (LOWER STATE)
C        ND= NUMBER OF DUNHAM COEFFICIENT GROUPS --
C            ONE FOR EACH OMEGA QUANTUM NUMBER
```

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```
C          ND1= THE MAX L VALUE FOR THE DUNHAM COEFFIENT MATRIX:
C               Y(L,J)
C          LWAV= MINIMUM WAVELENGTH CF SPECTRM (ANGSTRCMS)
C          LWAV1= MAXIMLM WAVELENGTH OF SPECTRUM (ANGSTROMS)
C          NROT= NUMBER OF POSSIBLE ROTATICNAL LEVELS
C     NOTE:   ALL INTEGERS USED TC DEFINE ARRAYS REFERING TO
C             VIBRATIONAL LEVELS ARE CNE LARGER THAN THE
C             CORRESPCNDING VIB. LEVEL.
C
      CHARACTER*45    NAMCEV
C
      CALL ASSIGN(3,'CHECK.OUT')
      WRITE(6,*) 'WHAT TYPE OF DEVICE DO YOU WANT TO PLOT ON?'
      WRITE(6,*) 'SPECIFY:    1       FCR HP 755C'
      WRITE(6,*) '            2       FCR TEKTRONIX 4107'
      WRITE(6,*) '            3       FCR VT240'
      WRITE(6,*) '            4       FOR VT 10C RETRO'
      WRITE(6,*) '            5       FCR TEKTRCNIX 401C'
      WRITE(6,*) '            6       FCR ANY ASCII PRINTER'
      READ(6,*) IPLOT
      IF(IPLCT.EC.1) NAMDEV='HP 7550'
      IF(IPLCT.EC.2) NAMCEV='TEKTRONIX 41C7'
      IF(IPLCT.E3.3) NAMCEV='VT 240'
      IF(IPLCT.EC.4) NAMCEV='VT 1CO RETRC'
      IF(IPLCT.EC.5) NAMCEV='TEKTRONIX 4C10'
      IF(IPLCT.EC.6) NAMCEV='ANY ASCII PRINTER'
      CALL PLTCEV(NAMCEV)
      CALL INPUT
      CALL INTENSE
      CALL OLTPUT
      CALL DCNEPL
      CALL CLOSE(3)
      STOP
      END
      SUBROUTINE INPUT
      PARAMETER(NROT=125)
      COMMCN/FACT/F(3,30,30),Y(9,3C,2),G(9,3C),
     1 G(9,3C),DG(9,3C)
      COMMCN/P    /TRW(6,30,30),P1(6,NROT),P2(6,NRCT),
     1 P1INT(6,NRCT),P2INT(6,NROT)
      COMMCN/G    /Q1(6,NROT),Q2(6,NRCT),
     1 Q1INT(6,NROT),Q2INT(6,NROT)
      COMMON/R    /R1(6,NROT),R2(6,NRCT),R1INT(6,NROT),
     1 R2INT(6,NROT),FINT(6,1C00C),FIN(1CC00),FINX(1CC00)
      COMMCN/TEMP/TV,TR
      COMMCN/INPLT/NTITLE,IFDIS,IBRANCH,WMIN,WMAX,RRES,
     1 XTV,XTR,IFDCNE,IFCEF,IPIN,IPAX,IENVH,ENVH1,V,
     2 XP,TK,GAMMA2
      COMMON/INDEX/NF,NF1,NF2,NT,ND,ND1
      COMMON/WGHT/WGHT(3C,30),NVIB,IFEXCIT
      COMMON/CNTR/CNTR(3,30,3C),IFCENTR
      COMMCN/EXPDAT/IFDATA,WAVE(2C,1C30),SPEC(20,103C),WAV(2CC00),
     1 SP(20CCO),WW(2COCC),SPW(2CCC0),WDAT(2C),SEN(2C),ICCUNT,IIMAX,
     2 INMAX,BKGFND,SLOPE
      COMMCN/PERT/IFPERT,TRP,IFPLE,VAR,VAR1,VAR2
      CHARACTER*4C    ATITLE
      CHARACTER*3C    IFILE
C
C
C READ IN THE APPROPRIATE FRANK CONDCN FACTORS
```

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```
C
      CALL ASSIGN(2,'FRANK.CON')
      READ(2,*) NF,NF1,NF2,NT
      WRITE(3,*) NF,NF1,NF2,NT
      DO 10 N=1,NF
C N=1 IMPLIES B1/2 -- X1/2 ELECTRONIC TRANSITION
C N=2 IMPLIES B3/2 -- X3/2 ELECTRONIC TRANSITION
      DO 20 I=1,NF1
      READ(2,*) (F(N,I,IF),IP=1,NF2)
      WRITE(3,*) (F(N,I,IP),IP=1,NF2)
  20    CONTINUE
  10    CONTINUE
      CLOSE(2)
C
C READ IN THE DUNHAM COEFFICIENTS
C
C NOTE: THE ZERO POINT ENERGIES ARE INCLUDED IN THE FIRST
C DUNHAM COEFFICIENT IN THIS FORMULATION
C
      CALL ASSIGN(2,'DUNHAM.COF')
      READ(2,*) ND,ND1
      WRITE(3,*) ND,ND1
      DO 30 M=1,ND
C M=1 IMPLIES X2PI1/2 STATE
C M=2 IMPLIES B2PI1/2 STATE
C M=3 IMPLIES X2PI3/2 STATE
C M=4 IMPLIES B2PI3/2 STATE
      DO 40 L=1,ND1
      READ(2,*) Y(M,L,1),Y(M,L,2)
  40    CONTINUE
      DO 39 L=1,ND1
      WRITE(3,*) Y(M,L,1),Y(M,L,2)
  39    CONTINUE
  30    CONTINUE
      CALL CLOSE(2)
      WRITE(6,*) 'IF YOU HAVE NOT DONE THIS SPECTRUM BEFORE OR WOULD',
     1 ' LIKE TO START FROM SCRATCH TYPE: 0 , OTHERWISE TYPE: 1 .'
      READ(6,*) IFDONE
      IF(IFDONE.EQ.0) THEN
       WRITE(6,*)'WHAT DO YOU WANT TO ENTITLE YOUR SPECTRUM?'
       READ(6,33) NTITLE
  33    FORMAT(A30)
       WRITE(6,*) 'IF YOU WANT THE CODE TO DETERMINE THE MINIMUM AND',
     2 ' MAXIMUM WAVELENGTHS BETWEEN WHICH THE SPECTRUM IS TO BE',
     3 ' PLOTTED TYPE: 0 ',
     4 ' NOTE: THIS RESOLVES THE SPECTRUM ON 2000 POINTS IN WAVELENGTH'
       READ(6,*) IFDEF
        IF(IFDEF.NE.0) THEN
         WRITE(6,*) 'WHAT IS THE MINIMUM WAVELENGTH(WMIN) IN ANGSTROM?'
         READ(6,*) WMIN
         WRITE(6,*) 'WHAT IS THE MAXIMUM WAVELENGTH(WMAX) IN ANGSTROM?'
         READ(6,*) WMAX
         WRITE(6,*) 'WHAT RESOLUTION(RES) DO YOU DESIRE IN THE SPECTM?'
         WRITE(6,*) 'NOTE:(WMAX-WMIN)/RES .LE. 10000 AND MUST BE AN',
     1               'INTEGER'
         READ(6,*) RRES
        ENDIF
       WRITE(6,*) 'WHAT IS THE VIBRATIONAL TEMPERATURE (DEG KELVIN)?'
       READ(6,*) XTV
       WRITE(6,*) 'WHAT IS THE ROTATIONAL TEMPERATURE (DEG KELVIN)?'
```

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```fortran
      READ(6,*) XTR
      WRITE(6,*) 'DC YOU WANT A LORENTZIAN (C) CR GAUSSIAN (1)',
     1 'DISTRIBUTION (GAUSSIAN NOT YET IMPLEMENTED)?'
      READ(6,*) IFDIS
      IF(IFDIS.EQ.0) THEN
       WRITE(6,*) 'WHAT IS GAMMA**2 FOR LORENTZIAN? IF C IS RETURNED',
     1 'GAMMA**2=9.5E'
       READ(6,*) GAMMA2
       IF(GAMMA2.EQ.C) THEN
        GAMMA2=9.58
       ENDIF
      ENDIF
      IF(IFDIS.EQ.1) THEN
       WRITE(6,*) 'WHAT IS THE GAS KINETIC TEMPERATURE (KELVIN)?'
       READ(6,*) TK
       WRITE(6,*) 'WHAT IS THE EMITTING MOLECULES MOLECULAR WEIGHT',
     1 '(GRAMS/MOLE)?'
       READ(6,*) XM
      ENDIF
      WRITE(6,*) 'WHAT IS THE EXPECTED ENVELOPE WIDTH OF THE',
     1 'THE DISTRIBUTION (IN ANGSTROMS)-- IF ZERO IS RETURNED THE',
     2 'CODE WILL ESTIMATE A VALUE.'
      READ(6,*) ENVH1
      WRITE(6,*) 'WHAT TYPE CF RCTATIONAL BRANCHING IS REQUIRED?'
      WRITE(6,*) ' THE CHOICES ARE: '
      WRITE(6,*) ' 1) P1,Q1,R1,P2,Q2,R2 FOR 2PI--2PI TRANSITIONS'
      WRITE(6,*) '    CCRRESPONDING TO HUNDS CASE A.'
      READ (6,*) IBRANCH
      WRITE(6,*) 'IF YOUR UPPER ELECTRONIC STATE HAS A NON-EQUILIBRIUM'
      WRITE(6,*) 'VIBRATIONAL DITRIBUTION TYPE: 1 '
      WRITE(6,*) '                    OTHERWISE TYPE: C '
      WRITE(6,*) 'HAVE THE RELATIVE WEIGHTS CF EACH VIBRATIONAL LEVEL'
      WRITE(6,*) 'IN FILE POPLTN.WT'
      READ(6,*) IFEXCIT
      IF(IFEXCIT.EQ.1) THEN
       CALL ASSIGN(2,'PCPLTN.WT')
       READ(2,*) NVIB
C NVIB IS THE NUMBER CF VIBRATIONAL LEVELS IN THE UPPER STATE YOU HAVE
C WEIGHTS FOR.  ALSO THERE IS ONE SET CF WEIGHTS FOR EACH TRANSITION.
       DO 5C N=1,NF
       READ(2,*) (WGHT(N,I),I=1,NVIB)
       WRITE(3,*) (WGHT(N,I),I=1,NVIB)
50     CONTINUE
       CALL CLOSE(2)
      ENDIF
       WRITE(6,*) 'IF YOU WANT TC WEIGHT THE SPECTRAL INTENSITIES'
       WRITE(6,*) 'WITH THE R-CENTRCIDS TYPE: 1 '
       WRITE(6,*) '                    OTHERWISE TYPE: 0'
       WRITE(6,*) 'THE R-CENTROIDS ARE ASSUMED TO BE IN RCENTROID.DAT'
       READ(6,*) IFCENTR
      IF(IFCENTR.EQ.1) THEN
       CALL ASSIGN(2,'RCENTRCID.DAT')
      DO 70 N=1,NF
C N=1 IMPLIES B1/2 -- X1/2 ELECTRONIC TRANSITION
C N=2 IMPLIES B3/2 -- X3/2 ELECTRONIC TRANSITION
C THERE SHOULD BE AS MANY R-CENTRCIDS AS FRANK-CONDON FACTORS
      DO 80 I=1,NF1
      READ(2,*) (CNTR(N,I,IP),IP=1,NF2)
      WRITE(3,*) (CNTR(N,I,IP),IP=1,NF2)
80    CONTINUE
```

```
70     CONTINUE
         CALL CLOSE(2)
       ENDIF
       WRITE(6,*) 'INCLUDE NON-BOLTZMANN CONTRIBUTION TC  ROTATIONAL'
       WRITE(6,*) 'LEVELS AS SPECIFIED BELOW ? YES (1), NC (0).'
       READ(6,*) IFPERT
       IF(IFPERT.EQ.1) THEN
         WRITE(6,*) 'WHAT IS THE FSEUDO RCTATICNAL TEMPERATURE (K)?'
         READ(6,*) TRF
         WRITE(6,*) 'WHAT IS THE RELAT HEIGHT CF 2ND EXP FCR RCT DIS?'
         READ(6,*) VAR
         WRITE(6,*) 'AT WHICH RCT. LINE DCES CCNT. TAKE EFFECT'
         READ(6,*) VAR1
         VAR2=VAR1-1
       ENDIF
       WRITE(6,*) 'PUBLICATICN QUALITY (GRAPHS BLACK)? YES (1), NC (0).'
       READ(6,*) IFPUE
       WRITE(6,*) 'DO YOU WANT TO PLOT THE THECRETICAL ANC EXPERIMENTAL'
       WRITE(6,*) 'SPECTRA ON THE SAME GRAFH? YES (1) , NC (0)'
       READ(6,*) IFDATA
       IF(IFDATA.EQ.1) THEN
       WRITE(6,*) 'SPECIFY THE THE AVERAGE NUMBER CF BACKGROUNC CCUNTS'
       WRITE(6,*) 'PER PIXEL TC SUBTRACT FROM YOUR DATA. CC THIS BY'
       WRITE(6,*) 'FIRST SPECIFYING THE INITIAL NUMBER CF COUNTS TC'
       WRITE(6,*) 'SUBTRACT AT YOUR MINIMUM WAVELENGTH'
       READ(6,*) EKGRNC
       WRITE(6,*) 'NCW SPECIFY THE SLCPE CF THE LINE CF THE'
       WRITE(6,*) 'AVERAGE INCREASE IN COUNTS/ANSTROM'
       READ(6,*) SLCPE
       WRITE(6,*) 'YCUR SFECTRAL CATA IS ASSUMED TC BE IN THE '
       WRITE(6,*) 'FILES NAMED IN : FILE.CMA.  NOTE THAT IT IS'
       WRITE(6,*) 'ALSC ASSUMED THAT THE FIRST FILE LISTED IN FILE.OMA'
       WRITE(6,*) 'CORRESPONDS TO THE LOWEST WAVELENGTH ANC SC ON '
       WRITE(6,*) 'IT IS ALSO ASSUMED THERE ARE NC GAPS IN WAVELENGTH'
       WRITE(6,*) 'BETWEEN CONSECUTIVE OMA FILES.'
       ENDIF
       IF(IFDATA.NE.1)THEN
         WRITE(6,*) 'CALCULATING THE SYNTHETIC SPECTRA...'
         WRITE(6,*) 'CRUNCH...CRUNCH...CRUNCH...'
       ENDIF
       ELSE
         WRITE(6,*) 'WHAT IS THE NAME CF YCUR INPUT FILE (TYPICALLY ',
     1   'INPUT.DAT)?'
         READ(6,35) IFILE
         CALL ASSIGN(2,IFILE)
         READ(2,*) WMIN,WMAX,RRES,XTV,XTR
         READ(2,35) NTITLE
35     FORMAT(A3C)
36     FORMAT(1X,A3C)
         READ(2,*) IFDIS,IBRANCH,ENVH1,TK,XM,GAMMA2
         READ(2,*) IFEXCIT,IFCENTR
         CALL CLOSE(2)
         WRITE(6,*) 'THE INPUT.CAT FILE HAS THE FOLLOWING VARIABLE',
     1   ' VALUES:'
         WRITE(6,*) 'THE PLOT TITLE IS                    1:'
         WRITE(6,36) NTITLE
         WRITE(6,*) 'LORENTZIAN(0) CR GAUSSIAN(1) DIS. 2:',IFDIS
         WRITE(6,*) 'THE ENVELOPE HALF WIDTH CF DIS.   3:',ENVH1
         WRITE(6,*) 'THE BRANCHING IS GIVEN BY'
         WRITE(6,*) '1) 2PI--2PI/HUNDS CASE A            4:',IBRANCH
```

```
      WRITE(6,*) 'THE MINIMUM WAVELENGTH(A) IS        5:',WMIN
      WRITE(6,*) 'THE MAXIMUM WAVELENGTH(A) IS        6:',WMAX
      IFDEF=1
      WRITE(6,*) 'THE MIN RESOLUTION IN ANGSTOMS      7:',RRES
      WRITE(6,*) 'THE VIBRATIONAL TEMP (KELVIN) IS    8:',XTV
      WRITE(6,*) 'THE ROTATIONAL TEMP (KELVIN) IS     9:',XTR
      IF(IFDIS.EQ.0) THEN
      WRITE(6,*) 'GAMMA**2 IS                        1C:',GAMMA2
      ENDIF
      IF(IFDIS.EQ.1) THEN
      WRITE(6,*) 'THE GAS KINETIC TEMP (KELVIN) IS 11:',TK
      WRITE(6,*) 'THE MOLECULAR WEIGHT (G/MOLE) IS 12:',XM
      ENDIF
      WRITE(6,*) 'THE UPPER STATE VIBRATIONAL LEVELS'
      WRITE(6,*) 'ARE IN EQUILIBRIUM (0) OR THEY ARE'
      WRITE(6,*) 'EXCITED (1)                      13:',IFEXCIT
      WRITE(6,*) 'INCLUDE R-CENTROIDS,YES(1),NO(C) 14:',IFCENTR
      WRITE(6,*) '***WHICH OF THE ABOVE VARIABLES DO YOU',
     1 ' WANT TO CHANGE? TYPE 0 WHEN YOU ARE FINISHED',
     2 ' MAKING CHANGES. ENTER NUMBERS ONE AT A TIME.'
      DO 15C I=1,14
      READ(6,*) IVAR
      IF(IVAR.EC.C) GO TO 16C
      IF(IVAR.EC.1) THEN
       WRITE(6,*) 'PLOT TITLE:'
       READ(6,35) NTITLE
      ENDIF
      IF(IVAR.EC.2) THEN
       WRITE(6,*) 'DISTRIBUTION (0 OR 1):'
       READ(6,*) IFDIS
       IF(IFDIS.EQ.C) THEN
       WRITE(6,*) 'REMEMBER TO MODIFY VARIABLES 11 AND 12'
       ENDIF
      ENDIF
      IF(IVAR.EC.3) THEN
       WRITE(6,*) 'ENVELOPE HALF WIDTH (ANGSTROMS):'
       READ(6,*) ENVH1
      ENDIF
      IF(IVAR.EC.4) THEN
       WRITE(6,*) 'BRANCHING IS:'
       READ(6,*) IBRANCH
      ENDIF
      IF(IVAR.EC.5) THEN
       WRITE(6,*) 'MIN WAVELENGTH (ANGSTROMS):'
       READ(6,*) WMIN
      ENDIF
      IF(IVAR.EQ.6) THEN
       WRITE(6,*) 'MAX WAVELENGTH (ANGSTROMS):'
       READ(6,*) WMAX
      ENDIF
      IF(IVAR.EQ.7) THEN
       WRITE(6,*) 'RESOLUTION (ANGSTROMS):'
       READ(6,*) RRES
      ENDIF
      IF(IVAR.EQ.8) THEN
       WRITE(6,*) 'VIB TEMPERATURE (KELVIN):'
       READ(6,*) XTV
      ENDIF
      IF(IVAR.EQ.9) THEN
       WRITE(6,*) 'ROT TEMPERATURE (KELVIN):'
```

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                   READ(6,*) XTR
                ENDIF
                IF(IVAR.EG.10) THEN
                 WRITE(6,*) 'GAMMA**2 IS:'
                 READ(6,*) GAMMA2
                ENDIF
                IF(IVAR.EG.11) THEN
                 WRITE(6,*) 'GAS KINETIC TEMPERATURE (KELVIN):'
                 READ(6,*) TK
                ENDIF
                IF(IVAR.EG.12) THEN
                 WRITE(6,*) 'MOLECULAR WEIGHT (GRAMS/MOLE):'
                 READ(6,*) XM
                ENDIF
                IF(IVAR.EG.13) THEN
                 WRITE(6,*) 'UPPERSTATE VIBRATIONAL EXCITATION'
                 WRITE(6,*) 'EQUILIBRIUM (C), NON-EQUILIBRIUM (1):'
                 READ(6,*) IFEXCIT
                ENDIF
                IF(IVAR.EG.14) THEN
                WRITE(6,*) 'INCLUDE R-CENTROIDS? YES(1) OR NO(C):'
                READ(6,*) IFCENTR
             ENDIF
  150      CONTINUE
  160      CONTINUE
           IF(IFEXCIT.EG.1) THEN
            CALL ASSIGN(2,'PCPLTN.WT')
            READ(2,*) NVIB
C NVIB IS THE NUMBER CF VIBRATIONAL LEVELS IN THE UPPER STATE YOU HAVE
C WEIGHTS FOR.  ALSO THERE IS CNE SET OF WEIGHTS FOR EACH TRANSITION.
            DO 60 N=1,NF
            READ(2,*) (WGHT(N,II),II=1,NVIB)
            WRITE(3,*) (WGHT(N,II),II=1,NVIB)
  60        CONTINUE
            CALL CLOSE(2)
           ENDIF
           IF(IFCENTR.EG.1) THEN
            CALL ASSIGN(2,'RCENTROID.DAT')
           DO 85 N=1,NF
C N=1 IMPLIES B1/2 -- X1/2 ELECTRONIC TRANSITION
C N=2 IMPLIES B3/2 -- X3/2 ELECTRONIC TRANSITION
C THERE SHOULD BE AS MANY R-CENTROIDS AS FRANK-CONDON FACTORS
           DO 90 II=1,NF1
           READ(2,*) (CNTR(N,II,IP),IF=1,NF2)
           WRITE(3,*) (CNTR(N,II,IP),IP=1,NF2)
  90       CONTINUE
  85       CONTINUE
            CALL CLOSE(2)
           ENDIF
           WRITE(6,*) 'INCLUDE NON-BOLTZMANN CONTRIBUTION TC  ROTATIONAL'
           WRITE(6,*) 'LEVELS AS SPECIFIED BELOW ? YES (1), NC (0).'
           READ(6,*) IFPERT
           IF(IFPERT.EG.1) THEN
             WRITE(6,*) 'WHAT IS THE PSEUDO ROTATIONAL TEMPERATURE (K)?'
             READ(6,*) TRF
             WRITE(6,*) 'WHAT IS THE RELAT HEIGHT CF 2ND EXP FCR RCT DIS?'
             READ(6,*) VAR
             WRITE(6,*) 'AT WHICH ROT. LINE DOES CCNT. TAKE EFFECT'
             READ(6,*) VAR1
             VAR2=VAR1-1
```

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      ENDIF
      WRITE(6,*) 'PUBLICATION QUALITY (GRAPHS BLACK)? YES (1), NC (0).'
      READ(6,*) IFPUE
      WRITE(6,*) 'DO YOU WANT TO PLOT THE THEORETICAL AND EXPERIMENTAL'
      WRITE(6,*) 'SPECTRA ON THE SAME GRAPH? YES (1) , NC (0)'
      READ(6,*) IFDATA
      IF(IFDATA.EQ.1) THEN
      WRITE(6,*) 'SPECIFY THE THE AVERAGE NUMBER OF BACKGROUND CCUNTS'
      WRITE(6,*) 'PER PIXEL TC SUBTRACT FROM YOUR DATA. DC THIS EY'
      WRITE(6,*) 'FIRST SPECIFYING THE INITIAL NUMBER OF COUNTS TO'
      WRITE(6,*) 'SUBTRACT AT YOUR MINIMUM WAVELENGTH'
      READ(6,*) BKGRNC
      WRITE(6,*) 'NOW SPECIFY THE SLOPE CF THE LINE CF THE'
      WRITE(6,*) 'AVERAGE INCREASE IN COUNTS/ANSTROM'
      READ(6,*) SLOPE
      WRITE(6,*) 'YOUR SPECTRAL DATA IS ASSUMED TC BE IN THE '
      WRITE(6,*) 'FILES NAMED IN : FILE.CMA.  NOTE THAT IT IS'
      WRITE(6,*) 'ALSC ASSUMED THAT THE FIRST FILE LISTED IN FILE.OMA'
      WRITE(6,*) 'CORRESPONDS TO THE LOWEST WAVELENGTH AND SC ON '
      WRITE(6,*) 'IT IS ALSO ASSUMED THERE ARE NC GAPS IN WAVELENGTH'
      WRITE(6,*) 'BETWEEN CONSECUTIVE OMA FILES.'
      ENDIF
      IF(IFDATA.NE.1)THEN
       WRITE(6,*) 'CALCULATING THE SYNTHETIC SPECTRA...'
       WRITE(6,*) 'CRUNCH...CRUNCH...CRUNCH...'
      ENDIF
      ENDIF
       TV=XTV*.695
       TR=XTR*.695
      IF(IFDIS.EC.1) THEN
       V=SQRT(2.494E8*TK/XM)*1E8
      ENDIF
      RETURN
      END
      SUBROUTINE INTENSE
      PARAMETER(NROT=125)
      COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
     1 B(9,30),DG(9,30)
      COMMON/P    /TR4(6,30,30),P1(6,NROT),P2(6,NRCT),
     1 P1INT(6,NROT),P2INT(6,NROT)
      COMMON/G    /Q1(6,NROT),Q2(6,NRCT),
     1 Q1INT(6,NRCT),G2INT(6,NROT)
      COMMON/R    /R1(6,NROT),R2(6,NRCT),R1INT(6,NROT),
     1 R2INT(6,NRCT),FINT(6,10000),FIN(10000),FINX(10000)
      COMMON/TEMP/TV,TR
      COMMON/INPUT/NTITLE,IFDIS,IERANCH,LMIN,LMAX,RRES,
     1 XTV,XTR,IFDONE,IFDEF,IMIN,IMAX,IENVH,ENVH1,V,
     2 XM,TK,GAMMA2
      COMMON/INDEX/NF,NF1,NF2,NT,ND,ND1
      COMMON/WGHT/WGHT(30,30),NVIB,IFEXCIT
      COMMON/CNTR/CNTR(3,30,30),IFCENTR
      COMMON/EXPDAT/IFDATA,WAVE(20,1030),SPEC(20,1030),WAV(20000),
     1 SP(20000),WW(20000),SPW(20000),WDAT(20),SEN(20),ICCUNT,IIMAX,
     2 INMAX,BKGRND,SLOPE
      COMMON/SPIN/NC
      CHARACTER*40   NTITLE

C
C
C    CALCULATE ENERGIES (G) AND MOLECULAR CONSTANTS (E) FOR
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C     VIBRATIONAL LEVELS
C
      NMAX=MAX(NF1,NF2)
      DO 10 M=1,ND
      DO 20 I=1,NMAX
      G(M,I)=0.
      B(M,I)=C.
      DO 30 L=1,ND1
C
      IEP=L-1
      XI=FLOAT(I)
      G(M,I)=G(M,I)+Y(M,L,1)*((XI-1.)+.5)**(IEP)
      B(M,I)=B(M,I)+Y(M,L,2)*((XI-1.)+.5)**(IEP)
C      WRITE(3,*) 'G,M,I=',G(M,I),M,I
  30  CONTINUE
      WRITE(3,*) 'G,M,I=',G(M,I),M,I
C
C     CALCULATE THE ENERGY DIFFERENCE (DG) BETWEEN VIBRATIONAL
C     LEVEL I AND THE LOWEST VIBRATIONAL LEVEL WITHIN THE ELECTRONIC STAT
C
      DG(M,I)=G(M,I)-G(M,1)
      WRITE(3,*) 'DG,M,I=',DG(M,I),M,I
C
  20  CONTINUE
  10  CONTINUE
C
C     CALCULATE THE VIBRATIONAL LEVEL TRANSITION (TR)
C     FREQUENCIES BETWEEN THE UPPER AND LOWER ELECTRONIC
C     LEVELS -- HUNDS CASE A.
C
      NN=1
      DO 40 N=1,NF
      DO 50 I=1,NF1
      DO 60 IP=1,NF2
      TRW(N,I,IP)=G(NN+1,I)-G(NN,IP)
      WRITE(3,*) 'TRANS',TRW(N,I,IP),N,I,IP
C     NOTE: BP-BPP<C FCR RED DEGRADED BANDS
C           BP-BPP>C FCR BLUE DEGRADED BANDS
      WRITE(3,*) 'BP-BPP=',B(NN+1,I)-B(NN,IP)
  60  CONTINUE
  50  CONTINUE
      NN=NN+2
  40  CONTINUE
C
C     DETERMINE THE MIN AND MAX EXTENT OF THE MESH IN ANGSTOMS
C     IF NOT SET IN THE INPUT
C
      IF(IFDEF.EC.0) THEN
      WMIN=1E20
      WMAX=C.
      DO 41 N=1,NF
      DO 51 I=1,NF1
      DO 61 IP=1,NF2
      XW=1.E8/TRW(N,I,IP)
      WMAX=MAX(XW,WMAX)
      WMIN=MIN(XW,WMIN)
  61  CONTINUE
  51  CONTINUE
  41  CONTINUE
      RRES=(WMAX-WMIN)/2C00.
```

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      ENDIF
      WRITE(3,*) 'RES=',RRES,'WMIN=',WMIN,'WMAX=',WMAX
      IF(ENVH1.EG.C.C) ENVH1=RRES*40.
      IENVH=INT(ENVH1/RRES)
      IMIN=INT((WMIN+.1*RRES)/RRES)-IENVH
      IMAX=INT((WMAX+.1*RRES)/RRES)+IENVH
      WRITE(3,*) 'ENVH1=',ENVH1,'IMIN=',IMIN,'IMAX=',IMAX
C
C     READ IN THE EXPERIMENTAL WAVELENGTHS AND PHOTON COUNTS IF
C     THE SYNTHETIC SPECTRUM IS TC BE COMPARED WITH EXPERIMENTAL
C     RESULTS.
C
      IF(IFDATA.EQ.1) THEN
       CALL LOADFIL
       WRITE(6,*) 'SPLICING AND CALIBRATING THE EXP SPECTRAL FILES...'
       CALL SPLICE
       CALL WEIGHT(WMIN,WMAX)
      WRITE(6,*) 'CALCULATING THE SYNTHETIC SPECTRA...'
      WRITE(6,*) 'CRUNCH...CRUNCH...CRUNCH...'
      ENDIF
C
C     FOR EACH VIBRATIONAL TRANSITION CALCULATE THE MULTITUDE CF
C     TRANSITIONS DUE TC ROTATIONAL SPLITTING CF THE VIBRATIONAL
C     LEVELS AND CALCULATE THE RELATED INTENSITIES.
C
      WMINE=WMIN-2*ENVH1
      WMAXE=WMAX+2*ENVH1
      NN=2
      DO 75 N=1,NF
C     THE EQUILIBRIUM POPULATION CF NS1/2 AND NS3/2 LEVELS
C     ARE NOT THE SAME.  THE RELATIVE NUMBER CF MOLECULES IN
C     EACH LEVEL IS EASILY DETERMINED USING THE ELECTRONIC
C     DISTRIBUTION FUNCTION.  AT 300 DEGREES KELVIN IT SHOWS
C     THAT IF THE POPULATION OF NS1/2 IS GIVEN BY 1, THEN THE
C     POPULATION CF NS3/2 IS GIVEN BY .6 .  THEREFORE, THE
C     N'S IN THE HERZBERG INTENSITY FORMULA DIFFER AS MENTIONED
C     ABOVE BETWEEN THE 1/2 AND 3/2 LEVELS.
      IF(N.EG.1)THEN
      FELEC=1.
      ELSE
      FELEC=.6
      ENDIF
C     DETERMINE THE NORMALIZATION FACTOR FOR BOLTZMAN
C     EQUILIBRIUM DISTRIBUTION OF POPULATIONS IN THE UPPER
C     STATE
      Z=C.
      DO 70 JJ=1,NF2-1
      Z=Z+EXP(-DG(NN,JJ)/TV)
70    CONTINUE
      DO 80 I=1,NF1
      DO 90 IP=1,NF2
      WIL=1.E8/TRW(N,I,IP)
      IF(WIL.LT.WMINE.OR.WIL.GT.WMAXE) GC TO 90
C
C     THIS IS THE NORMALIZED POPULATION FOR EACH VIBRATIONAL LEVEL
C     IN THE UPPER ELECTRONIC STATE
C
      IF(IFEXCIT.EQ.C) THEN
      EXPV=EXP(-DG(NN,I)/TV)/Z*FELEC
      WGHT(N,I)=EXPV
```

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      ENDIF
C
C     IF THERE IS A NCN-EQUILIBRIUM DISTRIBUTION OF
C     VIERATIONAL LEVELS THEY ARE SET HERE
C
      IF(IFEXCIT.EQ.1.AND.NVIB.GE.I) EXPV=WGHT(N,I)
C
C     IF ONE REQUIRES THE INCLUSICN CF THE R-CENTROIDS IN THE
C     COMPUTATION OF THE INTENSITIES THEIR CCNTRIEUTICN IS
C     TAKEN INTO ACCCUNT NEXT
C
      IF(IFCENTR.EG.1) THEN
      RE=-1.+1.76711*CNTR(N,I,IP)-1.C3755*CNTR(N,I,IP)**2
     1    +2.C28*CNTR(N,I,IP)**3
      EXPV=EXPV*RE**2
      ENDIF
C
C     THE LAMEDA TYPE COUELING OF EACH MULTIPLET(TWO CF THEM NC=1,2)
C     IS TAKEN INTC ACCOUNT IN THE NC LCCP.  THE EEFF CF THE FUNCTICNS
C     FP AND FPP CHANGE ACCORDINGLY.
C
      DO 72 NC=1,2
      IF(IERANCH.EQ.1) CALL DCUSLET(N,NN,I,IP,EXPV)
      WRITE(3,*) 'F,I,IP,EXPV=',F(N,I,IP),I,IF,EXPV
C
C     REDISTRIBUTE INTENSITIES WITH LCRENTZIAN -DUE TC HOMCGENEOUS SLIT
C     RELATED EROADENING
C
C     IF(IFDIS.EG.0) THEN
      CALL LORNTZN(N,I,IP)
 72   CONTINUE
 90   CONTINUE
 80   CONTINUE
      NN=NN+2
 75   CONTINUE
      RETURN
      END
      SUEROUTINE DOUELET(N,NN,I,IP,EXPV)
      PARAMETER(NROT=125)
      COMMCN/FACT/F(3,30,30),Y(9,30,2),G(9,30),
     1 B(9,30),DG(9,30)
      COMMCN/P   /TR4(6,30,30),P1(6,NROT),P2(6,NROT),
     1 P1INT(6,NRCT),F2INT(6,NROT)
      COMMON/G   /Q1(6,NROT),C2(6,NRCT),
     1 Q1INT(6,NRCT),C2INT(6,NROT)
      COMMCN/R   /R1(6,NROT),R2(6,NRCT),R1INT(6,NROT),
     1 R2INT(6,NRCT),FINT(6,1CCCC),FIN(1CCCC),FINX(1CCCC)
      COMMON/TEMP/TV,TR
      COMMCN/INPLT/NTITLE,IFDIS,IERANCH,WMIN,WMAX,RRES,
     1 XTV,XTR,IFDONE,IFDEF,IMIN,IMAX,IENVH,ENVH1,V,
     2 XM,TK,GAMMA2
      COMMCN/INDEX/NF,NF1,NF2,NT,ND,ND1
      DATA DE,DEP,AP,APP/1.2E-6,1.3E-6,149.7,285.8/
C  YY AND YE ARE THE LCWER AND UPPER STATE SPIN CRBIT SPLITTING
C  WAVE NUMBERS.
      DATA P,PE,YY,YE/1.,1.,221.5,90./
C     DATA F,PE,YY,YE/1.,1.,100CC,1CCOC/
      CHARACTER*40    ATITLE
      IF(N.EG.1) THEN
      Z=.5
```

```
          ZE=.5
          ELSE
          Z=1.5
          ZE=1.5
          ENDIF
          DO 100 J=1,NROT
          IF(N.EG.1) THEN
C N EQ 1 MEANS WE'RE COING BPI1/2--XPI1/2 TRANSITIONS
C P1-BRANCH
          R=FLOAT(J)-.5
          RE=R-1
          P1(N,J)=TRW(N,I,IP)+FP(R-1,NN,I,P,YE,DE)-FPP(R,NN,IP,F,YY,DEP)
          FR=P1(N,J)
C NOTE: THE COMPILER WAS HAVING A PROBLEM RECOGNIZING P1 IN THE
C XI FUNCTION CALL UNTIL I SET FR=P1(N,J) AND PASSED FR IN THE
C XI FUNCTION CALL, AS YOU SEE BELOW. BEFORE THE CHANGE, AT RUN
C TIME, FR WITHIN THE XI FUNCTION CALL WAS UNDEFINED = ZERO.
          CALL AINT(SJ,F,R,Z,YY,RE,PE,ZE,YE)
          P1INT(N,J)=XI(N,NN,I,IP,SJ,FR,RE,EXPV,YY)
C          WRITE(6,*) 'SJ OF P1=',SJ
C          WRITE(6,*) N,J,P1(N,J),P1INT(N,J)
C Q1-BRANCH
          RE=R
          Q1(N,J)=TRW(N,I,IP)+FP(R,NN,I,P,YE,DE)-FPP(R,NN,IP,P,YY,DEP)
          FR=Q1(N,J)
          CALL AINT(SJ,F,R,Z,YY,RE,PE,ZE,YE)
          Q1INT(N,J)=XI(N,NN,I,IP,SJ,FR,RE,EXPV,YY)
C R1-BRANCH
          RE=R+1.
          R1(N,J)=TRW(N,I,IP)+FP(R+1,NN,I,P,YE,DE)-FPP(R,NN,IP,P,YY,DEP)
          FR=R1(N,J)
          CALL AINT(SJ,P,R,Z,YY,RE,PE,ZE,YE)
          R1INT(N,J)=XI(N,NN,I,IP,SJ,FR,RE,EXPV,YY)
          ELSE
C N EG 2 MEANS WE'RE COING BPI3/2--XPI3/2 TRANSITIONS
C P2-BRANCH
          R=FLOAT(J)+.5
          RE=R-1.
          P2(N,J)=TRW(N,I,IP)+FP(R-1,NN,IP,P,YE,CE)-FPP(R,NN,IP,F,YY,DEP)
          FR=P2(N,J)
          CALL AINT(SJ,P,R,Z,YY,RE,PE,ZE,YE)
          P2INT(N,J)=XI(N,NN,I,IP,SJ,FR,RE,EXPV,YY)
C          WRITE(6,*) 'SJ OF P2=',SJ
C          WRITE(6,*) N,J,P2(N,J),FR,P2INT(N,J)
C Q2-BRANCH
          RE=R
          Q2(N,J)=TRW(N,I,IP)+FP(R,NN,IP,P,YE,DE)-FPP(R,NN,IP,P,YY,DEP)
          FR=Q2(N,J)
          CALL AINT(SJ,P,R,Z,YY,RE,PE,ZE,YE)
          Q2INT(N,J)=XI(N,NN,I,IP,SJ,FR,RE,EXPV,YY)
C R2-BRANCH
          RE=R+1.
          R2(N,J)=TRW(N,I,IP)+FP(R+1,NN,IP,F,YE,CE)-FPP(R,NN,IP,P,YY,DEP)
          FR=R2(N,J)
          CALL AINT(SJ,P,R,Z,YY,RE,PE,ZE,YE)
          R2INT(N,J)=XI(N,NN,I,IP,SJ,FR,RE,EXPV,YY)
          ENDIF
  100     CONTINUE
          RETURN
          END
```

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      REAL FUNCTION FF(R,NN,I,P,YE,DE)
      PARAMETER(NROT=125)
      COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
     1 B(9,30),DG(9,30)
      COMMON/P    /TRW(6,30,30),P1(6,NROT),P2(6,NROT),
     1 P1INT(6,NROT),P2INT(6,NROT)
      COMMON/SPIN/NC
      IF(P.LT.0) RETURN
      IF(NC.EQ.1)THEN
      BEFF=B(NN,I)*(1.+B(NN,I)/(P*ABS(YE)))
      ELSE
      BEFF=B(NN,I)*(1.-B(NN,I)/(P*ABS(YE)))
      ENDIF
      FP=BEFF*R*(R+1)-DE*R**2*(R+1)**2
      RETURN
      END
      REAL FUNCTION FFP(R,NN,IP,P,YY,DEP)
      PARAMETER(NROT=125)
      COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
     1 B(9,30),DG(9,30)
      COMMON/P    /TRW(6,30,30),P1(6,NROT),P2(6,NROT),
     1 P1INT(6,NROT),P2INT(6,NROT)
      COMMON/SPIN/NC
      IF(R.LT.0) RETURN
      IF(NC.EQ.1)THEN
      BEFF=B(NN-1,IP)*(1.+B(NN-1,IP)/(P*AES(YY)))
      ELSE
      BEFF=B(NN-1,IP)*(1.-B(NN-1,IP)/(P*AES(YY)))
      ENDIF
      FPF=BEFF*R*(R+1)-DE*R**2*(R+1)**2
C     IF(N.EQ.2) THEN
C     WRITE(6,*) 'N,NN,I,B(NN,I),B(NN-1,IP),R,PF'
C     WRITE(6,*) N,NN,I,B(NN,I),E(NN-1,IP),R,PF
C     ENDIF
      RETURN
      END
      REAL FUNCTION XI(N,NN,I,IP,SJ,FR,R,EXPV,YY)
      COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
     1 B(9,30),DG(9,30)
      COMMON/TEMF/TV,TR
      COMMON/PERT/IFPERT,TRP,IFPUB,VAR,VAR1,VAR2
      DATA P,DE /1,1.2E-6/
      IF(R.GE.0) THEN
      XI=B(NN,I)/TR*SJ*FR**3*F(N,I,IP)*
     1     EXP(-B(NN,I)*R*(R+1)/TR)*EXPV
      ELSE
      XI=0
      ENDIF
C DUE TO PERHAPS A SLOWLY RELAXING NASCENT DIST. OR PERHAPS
C DUE TO CURVE CROSSINGS(?) AT R VALUES GREATER THAN APPROXIMATELY
C 50 (SEE JEFFERIES) IN V' = 0,1 WE SEE ADDITIONAL PCPULATIONS
C IN THE HIGHER ROTATIONAL LEVELS. THIS EFFECT IS APPROXIMATED BY:
      IF(IFPERT.EQ.1)THEN
      IF(I.LE.2.AND.R.GE.VAR1) THEN
      XI=XI+VAR*B(NN,I)/TRP*SJ*FR**3*F(N,I,IP)*
     1     EXP(-B(NN,I)*(R-VAR2)*(R-VAR2+1)/TRP)*EXPV
      ENDIF
      ENDIF
C     IF(N.EQ.2) THEN
C     WRITE(6,*) 'N,NN,I,B(NN,I),SJ,FR,F(N,I,IP),EXPV,R'
```

```
C        WRITE(6,*) N,NN,I,B(NN,I),SJ,FR,F(N,I,IP),EXPV,R
C        ENDIF
         RETURN
         END
C
         SUBROUTINE AINT(SJ,P,R,Z,Y,RE,PE,ZE,YE)
C THIS SUBROUTINE CALCULATES THE ROTATIONAL LINE STRENGTHS FOR
C DOUBLET TRASNSITIONS.
C DEFINITION OF SYMBOLS IN AINT SUBROUTINE:
C   INPUT CONSTANTS (LOWER STATE IS A SINGLE LETTER: EXCITED STAT
C   HAS AN ADDED E):
C     R,RE - ROTATIONAL QUANTUM NUMBER, J (POSITIVE HALF INTEGER).
C              SELECTION RULE: DJ=0,1,-1
C     P,PE - ANGULAR MOMENTUM OF ELECTRONIC STATE, LAMDA (POSITIVE
C              INTEGER OR ZERO). SELECTION RULE: DLAMDA=C,1,-1
C     Z,ZE - TOTAL ANGLLAR MOMENTUM OF THE ELECTRONS, OMEGA
C              (HALF INTEGER = LAMDA + OR - .5)
C     Y,YE - DIMENSIONLESS SPIN ORBIT COUPLING CONSTANT,LAMDA.
C              PURE CASE A, LAMDA=1CC00.  PURE CASE B, LAMDA<E-5.
C   OUTPUT:
C     SJ - ROTATIONAL LINE STRENGTH FACTOR
C
         SJ=0.C
         SL=P-PE
         IF(ABS(SL)-1.01)1,1,35
  1      SR=R-RE
         IF(ABS(SR)-1.01)2,2,35
  2      IF(ABS(Y)-9999.C)5,5,3
  3      IF(ABS(YE)-9999.0)13,13,4
  4      IF(ABS(Z-ZE)-.C1)13,13,35
  5      IF(ABS(Y)-.000C2)6,6,13
  6      IF(ABS(YE)-.00CC2)7,7,13
  7      IF(ABS(R-Z)-.01)10,10,8
  8      IF(ABS(RE-ZE)-.C1)10,10,9
  9      IF(ABS(SR-SL+Z-ZE)-1.01)10,1C,35
 10      IF(P-.C1)11,11,13
 11      IF(PE-.01)12,12,13
 12      IF(ABS(SR+Z-ZE)-.01)35,35,13
 13      IF(R-Z+.01)35,14,14
 14      IF(RE-ZE+.C1)35,15,15
 15      AJ=RE+1.0
         S=P-.5
         SE=PE-.5
 16      IF(ABS(SL)-.01)23,17,17
 17      IF(ABS(SR)-.C1)18,21,21
 18      Q=.5*SGRT((AJ+SL*SE)*(RE-SL*SE)
        1 *(RE+AJ)/(RE*AJ))
         GO TO 27
 19      Q=.5*SGRT((AJ+1.+SL*SE)*(AJ+SL*SE)/AJ)
         GO TO 27
 2C      Q=SE*SGRT((AJ+RE)/(RE*AJ))
         GO TO 27
 21      IF(SR)22,19,19
 22      Q=.5*SGRT((RE-SL*S)*(AJ-SL*S)/RE)
         GO TO 27
 23      IF(ABS(SR)-.01)20,24,24
 24      IF(SR) 26,26,25
 25      Q=SQRT((AJ*AJ-SE*SE)/AJ)
         GO TO 27
 26      G=SQRT((RE*RE-S*S)/RE)
```

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```fortran
27      SI=1.0
        SK=1.0
        SIE=1.C
        SKE=1.C
        IF(ABS(Z-S)-.01)30,30,28
28      SI=-1.C
        IF(Z-S+.01)29,25,3C
29      SK=-1.C
30      IF(ABS(ZE-SE)-.C1)33,33,31
31      SIE=-1.C
        IF(ZE-SE+.C1)32,32,33
32      SKE=-1.C
33      S=S+1
        SE=SE+1
        SJ=SJ+T(SI,SK,P,R,Y)*Q*T(SIE,SKE,PE,RE,YE)
        IF(S-P-1.49)16,34,34
34      SJ=SJ*SJ
35      RETURN
        END
        REAL FUNCTICN T(SI,SK,P,R,Y)
        IF(P-.C1)6,6,1
 1      IF(R+.49-P)9,9,2
 2      AJ=2.*R+1.
        IF(ABS(Y)-.C00C2)8,8,3
 3      SL=Y/AES(Y)
        IF(ABS(Y)-9999.C)4,4,7
 4      GA=Y*P*P/AJ-R-.5
        GB=.5*SCRT(AJ**2+Y*(Y-4.)*F*P)
 5      BK=1./SCRT(2.*GE*AJ)
        T=BK*(SCRT((GB-SI*GA)*(R+.5-SL*P))+SI
       1*SQRT((GB+SI*GA)*(R+.5+SL*P)))*SK
        GO TO 10
 6      T=SI/SQRT(2.0)*SK
        GO TC 10
 7      GA=SL*P*P/AJ
        GB=.5*F
        GO TO 5
 8      T=SI*SK*SQRT((R+.5-SI*P)/AJ)
        GO TO 1C
 9      T=.5*SK*(1.+SI)
1C      RETURN
        END
        SUBROUTINE LCRNTZN(N,I,IP)
        PAPAMETER(NROT=125)
        COMMON/FACT/F(3,30,30),Y(9,3C,2),G(9,30),
       1 9(9,3C),DG(9,3C)
        COMMCN/P    /TRW(6,30,30),P1(6,NROT),P2(6,NROT),
       1 P1INT(6,NRCT),F2INT(6,NROT)
        COMMCN/G    /Q1(6,NROT),Q2(6,NRCT),
       1 Q1INT(6,NROT),C2INT(6,NROT)
        COMMON/R    /R1(6,NROT),R2(6,NRCT),R1INT(6,NROT),
       1 R2INT(6,NRCT),FINT(6,1C00C),FIN(1CCCC),FINX(1CCCC)
        COMMCN/TEMP/TV,TR
        COMMON/INPUT/NTITLE,IFDIS,IBRANCH,WMIN,WMAX,RRES,
       1 XTV,XTR,IFDCNE,IFCEF,IMIN,IMAX,IENVH,ENVH1,V,
       2 XP,TK,GAMMA2
        COMMON/INDEX/NF,NF1,NF2,NT,ND,ND1
        COMMCN/PEAK/XPEAK(6,30,30),YPEAK(6,30,3C),FCH(1C00C)
        CHARACTER*4C    NTITLE
C
```

```
C      NORPALIZED LCRENTZIAK--SLIGHT REDISTRIBUTION OF
C      INTENSITIES
C
C         GAMPA2=3.16E13*3.16E13
          IDIF=IPAX-IMIN
          IXN=3
          WIL=1.E8/TRW(N,I,IF)
          IF(WIL.LT.WMIN+ENVH) THEN
          IL=INT((WIL+.1*RRES)/RRES)-IMIN+1
          IU=IL+IENVH
          XN=WIL
          ELSE
          IL=INT((WIL+.1*RRES)/RRES)-IMIN-IENVH+1
          IU=IL+2*IENVH
          XN=WIL-IENVH*RRES
          ENDIF
          WRITE (3,*) 'IL=',IL,'IU=',IU
          FMAX=C
          FMAX1=C
          FMAXCLD=0
          FMP=C
          RR=C.
          DO 110 I1=IL,IU
          IF(I1.LT.1.CR.I1.GT.IDIF)GO TO 110
          RR=RR+RRES
          XI1=XN+RR
C         XI1I=3.E18/XI1
          SUP=C
          IF(N.EC.1) THEN
          DO 120 J=1,NRCT
          DENOP=(XI1-1E8/F1(N,J))**2+GAMPA2
          SC=GAMPA2/DENCP
          SUP=SUP+SC*P1INT(N,J)
  120     CONTINUE
          DO 130 J=1,NROT
          DENCP=(XI1-1.E8/R1(N,J))**2+GAPPA2
          SC=GAPPA2/DENOP
          SUP=SUP+SC*R1INT(N,J)
  130     CONTINUE
          DO 140 J=1,NRCT
          DENOP=(XI1-1.E8/Q1(N,J))**2+GAPPA2
          SC=GAMPA2/CENOP
          SUP=SUP+SC*G1INT(N,J)
  140     CONTINUE
          ELSE
          DO 150 J=1,NRCT
          DENOM=(XI1-1.E8/P2(N,J))**2+GAPPA2
          SC=GAMPA2/CENOP
          SUP=SUP+SC*P2INT(N,J)
  150     CONTINUE
          DO 160 J=1,NRCT
          DENOP=(XI1-1.E8/R2(N,J))**2+GAPPA2
          SC=GAMPA2/DENOP
          SUP=SUP+SC*R2INT(N,J)
  160     CONTINUE
          DO 170 J=1,NRCT
          DENCM=(XI1-1.E8/G2(N,J))**2+GAPPA2
          SC=GAMPA2/CENCP
          SUP=SUP+SC*G2INT(N,J)
  170     CONTINUE
```

```
         ENDIF
          FIN(I1)=FIN(I1)+SUM
          FCH(I1)=SUM
C         WRITE(6,*) 'DEN=',DENCM,SC,GAMMA2,Q2INT(N,J),SUM
C   FIND THE MAX Y POSITION OF "CLOSE" PEAKS
          FMAX=MAX(FIN(I1),FMAX)
          FMAX1=MAX(FCH(I1),FMAX1)
          IF(FMAX.GT.FMAXOLD.AND.(FMAX1/FMAX).GT..2) THEN
           FMAXOLD=FMAX
           YPEAK(N,I,IP)=MAX(YPEAK(N,I,IP),FMAX)
          ENDIF
  110   CONTINUE
C
C       END OF INTEGRATION
C
C
C       FIND THE PEAK OF EACH SPECTRUM LINE
C
        FMAX=0
        FMAX1=0
        FMAXOLD=0
        RR=0.
        IL=INT((WIL+.1*RRES)/RRES)-IMIN-IXN+1
        IU=IL+2*IXN
        XN=WIL-IXN*RRES
        DO 5 I1=IL,IU
        IF(I1.LT.1.OR.I1.GT.IDIF)GO TO 5
        RR=RR+RRES
        XI1=XN+RR
         FMAX=MAX(FIN(I1),FMAX)
         FMAX1=MAX(FCH(I1),FMAX1)
         IF(FMAX.GT.FMAXOLD.AND.(FMAX1/FMAX).GT..2) THEN
          XPEAK(N,I,IP)=XI1
          YPEAK(N,I,IP)=MAX(YPEAK(N,I,IP),FMAX)
          FMAXOLD=FMAX
         ENDIF
  5     CONTINUE
        RETURN
        END
        SUBROUTINE GAUSSN(N,I,IP)
        PARAMETER(NROT=125)
        COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
       1 B(9,30),DG(9,30)
        COMMON/P    /TRW(6,30,30),P1(6,NROT),P2(6,NROT),
       1 P1INT(6,NROT),P2INT(6,NROT)
        COMMON/Q    /Q1(6,NROT),Q2(6,NROT),
       1 Q1INT(6,NROT),Q2INT(6,NROT)
        COMMON/R    /R1(6,NROT),R2(6,NROT),R1INT(6,NROT),
       1 R2INT(6,NROT),FINT(6,10000),FIN(10000),FINX(10000)
        COMMON/TEMP/TV,TR
        COMMON/INPUT/NTITLE,IFDIS,IBRANCH,WMIN,WMAX,RRES,
       1 XTV,XTR,IFDONE,IFDEF,IMIN,IMAX,IENVH,ENVH1,V,
       2 XM,TK,GAMMA2
        COMMON/INDEX/NF,NF1,NF2,NT,ND,ND1
        COMMON/PEAK/XPEAK(6,30,30),YPEAK(6,30,30),FCH(10000)
        CHARACTER*40    NTITLE
C
C       NORMALIZED GAUSSIAN
C
        RETURN
```

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```fortran
      END
      SUBROUTINE OUTPLT
      PARAMETER(NROT=125)
      COMMON/FACT/F(3,30,30),Y(9,30,2),G(9,30),
     1 B(9,30),DG(9,30)
      COMMON/P    /TRW(6,30,30),P1(6,NROT),P2(6,NROT),
     1 P1INT(6,NROT),P2INT(6,NROT)
      COMMON/G    /Q1(6,NROT),Q2(6,NROT),
     1 Q1INT(6,NROT),Q2INT(6,NROT)
      COMMON/R    /R1(6,NROT),R2(6,NROT),R1INT(6,NROT),
     1 R2INT(6,NROT),FINT(6,10000),FIN(10000),FINX(10000)
      COMMON/TEMP/TV,TR
      COMMON/INPLT/NTITLE,IFDIS,IERANCH,WMIN,WMAX,PRES,
     1 XTV,XTR,IFDONE,IFDEF,IPIN,IMAX,IENVH,ENVH1,V,
     2 XP,TK,GAMMA2
      COMMON/INDEX/NF,NF1,NF2,NT,ND,ND1
      COMMON/PEAK/XPEAK(6,30,30),YPEAK(6,30,30),FCH(10000)
      COMMON/WGHT/WGHT(30,30),NVIB,IFEXCIT
      COMMON/CNTR/CNTR(3,30,30),IFCENTR
      COMMON/EXPDAT/IFDATA,WAVE(20,1030),SPEC(20,1030),WAV(20000),
     1 SF(20000),WW(20000),SPW(20000),WDAT(20),SEN(20),ICOUNT,IIMAX,
     2 INMAX,BKGRND,SLOPE
      COMMON/PERT/IFPERT,TRP,IFPLE,VAR,VAR1,VAR2
      DIMENSION FINY(10000),YMAXX(30,30)
      CHARACTER*40    NTITLE
C
C
      CALL ASSIGN(7,'OUTPUT.SPEC')
C
C     WRITE INPUT FILE FOR CONTINUATION RUNS
C
      CALL ASSIGN(2,'INPUT.DAT')
      WRITE(2,*) WMIN,WMAX,PRES,XTV,XTR
      WRITE(2,35) NTITLE
  35  FORMAT(A30)
      WRITE(2,*) IFDIS,IERANCH,ENVH1,TK,XP,GAMMA2
      WRITE(2,*) IFEXCIT,IFCENTR
      CALL CLOSE(2)
C
C     NORMALIZE INTENSITY
C
      YMAX=0.
      YMIN=1.E20
      LMN=IMAX-IPIN
      LMNN=LMN-2*IENVH
C      DO 10 I=1,LMNN
      DO 10 I=IENVH,LMN-IENVH
      YMAX=MAX(FIN(I),YMAX)
      YMIN=MIN(FIN(I),YMIN)
  10  CONTINUE
      YM=YMAX
      II=0
      WMEN=WMIN-ENVH1
C      DO 20 I=1,LMNN
      DO 20 I=IENVH,LMN-IENVH
      II=II+1
      FINX(II)=WMEN+FLOAT(I-1)*PRES
      FINY(II)=FIN(I)/YMAX
      WRITE(7,*) FINX(II),FINY(II)
```

```
 20     CONTINUE
C
C       NORMALIZE PEAK INTENSITIES
C
        DO 25 N=1,NT
        DO 24 I=1,NF1
        DO 23 IP=1,NF2
        YPEAK(N,I,IF)=YPEAK(N,I,IP)/YMAX
 23     CONTINUE
 24     CONTINUE
 25     CONTINUE
        YMIN=YMIN/YMAX
        YMAX=1.
C
C       PLOT THE INTENSITY SPECTRUM AS A FUNCTION OF WAVELENGTH IN
C       ANGSTROMS USING DISSPLA.
C
        TTV=TV/.695
        TTR=TR/.695
C       XLWAV=WMIN-ENVH1
C       XLWAV1=WMAX+ENVH1
        XLWAV=WMIN
        XLWAV1=WMAX
        CALL PAGE(11,8.5)
        CALL AREA2D(10,6.5)
        NCHAR=INDEX(NTITLE,'             ')
        CALL HEADIN(XREF(NTITLE),NCHAR,2.,1)
        CALL XNAME('WAVELENGTH (ANGSTROMS)$',100)
        CALL YNAME('NORMALIZED INTENSITY$',100)
        CALL GRAF(XLWAV,'SCALE',XLWAV1,YMIN,'SCALE',YMAX)
        CALL MESSAG('ROT TEMP=$',100,7.35,6.25)
        CALL REALNO(TTR,-4,'ABUT','ABUT')
        CALL DASH
        CALL CURVE(FINX,FINY,LMNN,0)
        CALL RESET('DASH')
        WRITE(3,*)'IFDATA,IFEXCIT=',IFDATA,IFEXCIT
        IF(IFEXCIT.EQ.0)THEN
        NVIB=12
        CALL MESSAG('VIB TEMP=$',100,7.35,6.0)
        CALL REALNO(TTV,-4,'ABUT','ABUT')
          IF(IFDATA.EQ.0) THEN
          CALL MESSAG('V   1/2-1/2PCP 3/2-3/2POP$',100,7.35,5.75)
          YPOS=5.5
          DO 200 JJ=1,NVIB
          XPOS=7.35
          CALL INTNO(JJ-1,XPOS,YPOS)
          XPOS=XPOS+.3125
          CALL REALNO(WGHT(1,JJ),-2,XPOS,YPOS)
          XPOS=XPOS+1.3
          CALL REALNO(WGHT(2,JJ),-2,XPOS,YPOS)
          YPOS=YPOS-.2
 200      CONTINUE
          ELSE
          CALL MESSAG('-- SYNTHETIC SPECTRUM$',100,7.35,5.75)
          CALL MESSAG('V   1/2-1/2PCP 3/2-3/2POP$',100,7.35,5.25)
          YPOS=5.0
          DO 210 JJ=1,NVIB
          XPOS=7.35
          CALL INTNO(JJ-1,XPOS,YPOS)
          XPOS=XPOS+.3125
```

```
            CALL REALNO(WGHT(1,JJ),-2,XPOS,YPOS)
            XPOS=XPOS+1.3
            CALL REALNO(WGHT(2,JJ),-2,XPOS,YPOS)
            YPOS=YPOS-.2
  210       CONTINUE
            IF(IFPUB.EQ.C) THEN
            CALL SETCLR('RED')
            ENDIF
            CALL MESSAG(' - EXPER. SPECTRUMS',100,7.35,5.5)
C            CALL MARKER(15)
C            CALL SCLPIC(.7)
C            CALL CURVE(WW,SPW,INMAX,INMAX/1CC)
            CALL CURVE(WW,SPW,INMAX,C)
            WRITE(7,*) 'EXP WAVELENGTH , EXP FHOTCN CCUNTS'
            DO 27 II=1,INMAX
            WRITE(7,*) WW(II),SPW(II)
  27        CONTINUE
          ENDIF
        ENDIF
        IF(IFEXCIT.EQ.1) THEN
          IF(IFCATA.EQ.C) THEN
          CALL MESSAG('V  1/2-1/2PCP 3/2-3/2PCP1',100,7.35,6.0)
          YPOS=5.75
          CO 3CC JJ=1,NVIB
          XPOS=7.35
          CALL INTAC(JJ-1,XPOS,YPOS)
          XPOS=XPOS+.3125
          CALL REALNO(WGHT(1,JJ),-2,XPOS,YPOS)
          XPOS=XPOS+1.3
          CALL REALNO(WGHT(2,JJ),-2,XPOS,YPOS)
          YPOS=YPOS-.2
  300     CONTINUE
          ELSE
          CALL MESSAG('-- SYNTHETIC SPECTRUMS',100,7.35,6.C)
          CALL MESSAG('V  1/2-1/2PCP 3/2-3/2POPS',1C0,7.35,5.5)
          YPOS=5.25
          DO 31C JJ=1,NVIB
          XPOS=7.35
          CALL INTAC(JJ-1,XPOS,YPOS)
          XPOS=XPOS+.3125
          CALL REALNO(WGHT(1,JJ),-2,XPOS,YPOS)
          XPOS=XPOS+1.3
          CALL REALNO(WGHT(2,JJ),-2,XPOS,YPOS)
          YPOS=YPOS-.2
  310     CONTINUE
          IF(IFPUB.EQ.C)THEN
          CALL SETCLR('RED')
          ENDIF
          CALL MESSAG(' - EXPER. SPECTRUMS',100,7.35,5.75)
C            CALL MARKER(15)
C            CALL SCLPIC(.7)
          CALL CURVE(WW,SPW,INMAX,C)
          WRITE(7,*) 'EXP WAVELENGTH , EXP FHOTCN CCUNTS'
          DO 127 II=1,INMAX
          WRITE(7,*) WW(II),SPW(II)
  127     CONTINUE
          ENDIF
        ENDIF
        CALL HEIGHT(.C8)
        CALL ANGLE(90.)
```

37

```
              XN=1.7*.007353*(WMAX-WMIN)
              YN=.025
              CALL SETCLR('BLLE')
C      FINC WHERE LINE TRANSITICN NUMBERS WILL CVERLAP AND ELLIPNATE THE
C      CVERLAPPING NUMBERS
              N=1
              NN=2
              DO 40 I=1,NF1
              DO 50 IP=1,NF2
                 IF(AES(XPEAK(N,I,IP)-XPEAK(NN,I,IP)).LT.XN)THEN
                 WRITE(3,*) 'ABS(XP1/2-XF3/2),XN,I,IF=',ABS(XFEAK(N,I,IP)-
     1                      XPEAK(NN,I,IP)),XN,I,IP
                 YPEAK(NN,I,IF)=YPEAK(NN,I,IF)+1C
                 WRITE(3,*) 'YPEAK(2,I,IF)=',YPEAK(NN,I,IP)
                 ENDIF
   50     CONTINUE
   40     CONTINUE
C      WRITE THE NCN-OVERLAPPING NLMBERS CN THE PLCT
              N=1
              DC 60 I=1,NF1
              DC 70 IP=1,NF2
              IF(XLWAV.GT.XPEAK(N,I,IP).CR.XLWAV1.LT.XPEAK(N,I,IP))
     1    GC TC 70
              IF(YPEAK(N,I,IF).LT..001) GC TC 7C
              IC=I-1
              IFO=IF-1
              XMESS=XPEAK(N,I,IF)
              YMESS=1.+YN
              CALL RLMESS('(',1,XMESS,YMESS)
              CALL RLINT(IO,'ABLT','ABUT')
              CALL RLMESS(',',1,'ABUT','ABUT')
              CALL RLINT(IPC,'AEUT','ABUT')
              CALL RLMESS(')1/2$',10C,'AEUT','AEUT')
   70     CONTINUE
   60     CONTINUE
              N=2
              DC 80 I=1,NF1
              DC 90 IP=1,NF2
              IF(XLWAV.GT.XPEAK(N,I,IP).CR.XLWAV1.LT.XPEAK(N,I,IP))
     1    GO TC 90
              IF(YPEAK(N,I,IP).LT..001) GC TC 90
              IF(YPEAK(N,I,IP).LT.8) THEN
              IC=I-1
              IPO=IP-1
              XMESS=XPEAK(N,I,IF)
              YMESS=1.+YN
              CALL RLMESS('(',1,XMESS,YMESS)
              CALL RLINT(IC,'ABLT','ABUT')
              CALL RLMESS(',',1,'ABUT','ABUT')
              CALL RLINT(IPC,'ABUT','ABLT')
              CALL RLMESS(')3/2$',1CC,'AEUT','ABLT')
              ENDIF
   90     CONTINUE
   80     CONTINUE
              CALL RESET('HEIGHT')
              CALL RESET('ANGLE')
              CALL ENDPL(-1)
C
              RETURN
              END
```

```
      SUBROUTINE PLTDEV (NAMDEV)
**************************************************************
*
*                    (DEFINE    SUBROUTINE    HERE    !!!)
*
**************************************************************
*
*        WRITTEN EY:
*
*
*                         FRANK J. SEILER RESEARCH LABCRATCRY
*                         LNITEC STATES AIR FORCE ACADEPY
*                         COLORADO SPRINGS, COLCRADC  2C84C
*
**************************************************************
*    INPUT PARAMETERS:
*        NAMDEV  - OUTFUT DEVICE CHCSEN BY USER
*------------------------------------------------------------
         CHARACTER*45    NAMDEV
**************************************************************
*    LOCAL VARIABLES:
*        IBUF     -
*        IERR     - ERPCR NUMBER
*------------------------------------------------------------
         INTEGER         IBUF,I,II,IERR
         DIMENSION       IBUF(16)
**************************************************************
         CHARACTER       EELL
         BELL = CHAR(7)
*    TERMINAL DEVICES
         IF (NAMDEV .EC. 'VT 240') GOTC 21CO
         IF (NAMDEV .EC. 'TEKTRONIX 41U7') GCTC 22CO
         IF (NAMDEV .EC. 'TEKTRONIX 4C10') GOTC 23CO
         IF (NAMDEV .EC. 'VT 1CO RETRC') GCTO 240C
*    HARDCOPY DEVICES
         IF (NAMDEV .EC. 'PRINTRONICS') GCTO 31CO
         IF (NAMDEV .EC. 'HP 7550') GCTO 320C
         IF (NAMDEV .EO. 'HP 7475') GCTO 3300
         IF (NAMDEV .EC. 'ANY ASCII PRINTER') GOTC 34CC
         IF (NAMDEV .EC. 'PCST PRCCESSOR') GOTC 41CO
*    ERROR, QUIT
         GOTO 910C
*------------------------------------------------------------
*   TERMINAL DEVICES
*------------------------------------------------------------
*   VT 24C

2100     CONTINUE

*   SET CCNFIGURATICN TO STANDARD I/O
         IBUF(1)=C
         CALL IOMGR(IBUF,-102)

         CALL VT240

         GOTO 990CC
*------------------------------------------------------------
*   TEKTRONIX 41C7

2200     CONTINUE
```

```
*    SET CONFIGURATION TO STANDARD I/O
         IBUF(1)=C
         CALL IOMGR(IBLF,-102)

         CALL TK41 (4107)

*        PLOT ORIENTATION -        AUTO : AUTO ACCORDING TO PLT SIZE
*                                  CCMIC: X AXIS HORIZONTAL
*                                  MCVIE: Y AXIS HORIZONTAL
C        CALL HWROT('CCMIC')

         GOTO 99000
*---------------------------------------------------------------
*    TEKTRONIX 4010

2300     CONTINUE

         CALL P401C

         GOTO 99000
*---------------------------------------------------------------
*    VT 102 WITH GRAPHICS RETROFIT

2400     CONTINUE
*    SET CONFIGURATION TO STANDARD I/C
*        IBUF(1)=C
         CALL IOMGR(IBLF,-102)

         CALL PDEVT

         GOTO 99000
*---------------------------------------------------------------
*

2500     CONTINUE

         GOTO 99000
*---------------------------------------------------------------
*

2600     CONTINUE

         GOTO 99000
*---------------------------------------------------------------
*

2700     CONTINUE

         GOTO 99000
*---------------------------------------------------------------
*    HARDCOPY DEVICES
*---------------------------------------------------------------
*    PRINTRONICS

3100     CONTINUE

         CALL PPNTNX

         GOTO 99000
*---------------------------------------------------------------
```

```fortran
*   HP 7550

3200      CONTINUE

*   SET CCNFIGURATION TO SPOOL
          IBUF(1)=5
          CALL IOMGR(IELF,-102)

*     SET FILE CPEN MCDE
*                  3 - NC CVERWRITE, CREATES NEW VERSION NUMBER
*                  0 - APFEND TO FILE
          IBUF(1)=3
          CALL IOMGR(IELF,-1C4)

*   SET PLOT FILE NAME
          DO 3220 II=1,16
          IBUF(II)=C
322C      CONTINUE

          PRINT '(/////)'
3240      CONTINUE
          PRINT '(''S'',
     +              '' ENTER PLOT FILE NAME OR Q TO QUIT: '',A)', BELL
          READ(5, '(14A4)', ERR=93CC) (IBUF(II), II=1, 14)
C         IF (IBUF(1) .EQ. )

          CALL IOMGR(IELF,-1C3)

          CALL HP7550 (1)

*         FLOT CRIENTATION -        ALTO : ALTO ACCORDING TO PLT SIZE
*                                   CCMIC: X AXIS HORIZONTAL
*                                   MCVIE: Y AXIS HORIZONTAL
C         CALL HWRCT('MCVIE')

          GCTO 99CCC
*----------------------------------------------------------------
*   HP 7475

330C      CONTINUE

*   SET CCNFIGURATION TO SPOOL
          IBUF(1)=5
          CALL ICMGR(IELF,-1C2)

*     SET FILE CPEN MCDE
*                  3 - NO CVERWRITE, CREATES NEW VERSION NLMBER
*                  0 - APFEND TO FILE
          IBUF(1)=3
          CALL IOMGR(IELF,-1C4)

*   SET PLOT FILE NAME
          DC 3320 II=1,16
          IBUF(II)=C
3320      CCNTINUE

          PRINT '(/////)'
3340      CONTINUE
          PRINT '(''S'',
     +              ''                    ENTER PLOT FILE NAME: '',A)', BELL
```

```
          READ(5, '(14A4)', ERR=9400) (IBUF(II), II=1, 14)
          CALL ICMGR(IBLF,-103)

          CALL HP7475 (1)

*         PLOT ORIENTATION -        AUTO :  AUTO ACCORDING TO PLT SIZE
*                                   COMIC: X AXIS HORIZONTAL
*                                   MOVIE: Y AXIS HORIZONTAL
C         CALL HWROT('MOVIE')

          GOTO 99000
*------------------------------------------------------------------
*   ANY ASCII PRINTER         .

3400      CONTINUE

          CALL FPRTPL

          GOTO 99000
*------------------------------------------------------------------
*  POST PROCESSOR
*------------------------------------------------------------------
4100      CONTINUE

          CALL COMPRS

          GOTO 99000
*------------------------------------------------------------------

*   ERROR HANDLING    *********************************************

*   DEVICE SELECTION ERROR   ----------------
9100      PRINT '(''0'',
     +          21X, ''  *** ERROR IN PLOT DEVICE SELECTION ***'',
     +          A, A, A)', BELL, BELL, BELL
          STOP

*   HP 7550 FILE NAME ERROR ----------------
9300      PRINT '(''0'',
     +          21X, ''  *** ERROR IN FILE NAME ***'', A, /,
     +          21X, ''        PRESS RETURN'', A, A)', BELL, BELL, BELL
          READ(5, '(I1)', IOSTAT=IERR) I
          GOTO 3240

*   HP 7475 FILE NAME ERROR ----------------
9400      PRINT '(''0'',
     +          21X, ''  *** ERROR IN FILE NAME ***'', A, /,
     +          21X, ''        PRESS RETURN'', A, A)', BELL, BELL, BELL
          READ(5, '(I1)', IOSTAT=IERR) I
          GOTO 3340


99000     CONTINUE
          RETURN
          END
C
C*****************************************************************
          SUBROUTINE LOADFIL
C
C   THIS LOADS THE OPA FILES THAT INCLUDE WAVELENGTH INFORMATION
```

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```
C     IT ALSO PLACES THE WAVELENGTH AND CORRESPONDING INTENSITY DATA
C     IN FILES TO BE MANIPULATED IN SUBROUTINE SPLICE.  IT IS ASSUMED
C     THAT THE CMA FILES TO BE PLOTTED ARE PRESENT IN THE LOCAL FILE
C     SPACE AND LISTED IN FILE FILE.CMA.
C
      COMMON/EXPDAT/IFDATA,WAVE(20,1030),SPEC(20,1030),WAV(20000),
     1 SP(20000),WW(20000),SPW(20000),WDAT(20),SEN(20),ICOUNT,IIMAX,
     2 INMAX,BKGRND,SLOPE
      COMMON/COF/ACOF(20,50)
         CHARACTER*6 SHOTNO, SPC
         CHARACTER*4 END
         CHARACTER*10 SNODAT,FILES
         CHARACTER*20 CDUMMY1,CDUMY1
C
C
         DUMMY=0
         ICOUNT=0
         FILES='FILE.CMA'
         CALL ASSIGN(4,FILES)
         WRITE(6,*) 'LOADING FILES (NAMED IN FILE.CMA):'
         DO 100 I=1,20
               READ(4,101,END=9) SHOTNO
               ICOUNT=ICOUNT+1
               WRITE(6,*) I,' FILE= ',SHOTNO
               INUM=I
  101          FORMAT (A6)
               END='.CMA'
               SNODAT=SHOTNO//END
               CALL ASSIGN(2,SNODAT)
         READ(2,102) CDUMY1
  102    FORMAT(A19)
         DO 10 II=1,3
         READ(2,103) CDUMY2
  103    FORMAT(A11)
   10    CONTINUE
               DO 200 J=1,1024
               READ(2,*,END=201) SPEC(I,J)
  200          CONTINUE
  201          CONTINUE
         READ(2,102) CDUMY1
         DO 20 II=1,3
         READ(2,103) CDUMY2
   20    CONTINUE
               DO 210 J=1,40
               READ(2,*,END=211) ACOF(I,J)
  210          CONTINUE
  211          CONTINUE
               CALL CLOSE(2)
C        WRITE(3,*) 'EXP WAVE LEN , EXP PHOTON COUNT'
         DO 220 J=1,1024
         WAVE(I,J)=ACOF(I,36)+ACOF(I,37)*(FLOAT(J)-1.)
C        WRITE(3,*) WAVE(I,J),SPEC(I,J)
  220    CONTINUE
  100          CONTINUE
    9    CONTINUE
         CALL CLOSE(4)
         RETURN
         END
C
      SUBROUTINE SPLICE
```

```fortran
C     THIS SUBROUTINE SPLICES TOGETHER CMA FILES.  IT IS ASSUMED
C     THAT THE DATA FILES OVERLAP EACH OTHER AND THAT THEY ARE
C     NAMED IN FILE FILE.CMA.  IT IS ALSO ASSUMED THAT THE FIRST FILE
C     NAMED CORRESPONDS TO THE SHORTEST WAVELENGTH AND SO ON.
C
      COMMON/EXPDAT/IFDATA,WAVE(20,1030),SPEC(20,1030),WAV(20000),
     1 SP(20000),WW(20000),SPW(20000),WDAT(20),SEN(20),ICOUNT,IIMAX,
     2 INMAX,BKGRND,SLOPE
      COMMON/COF/ACOF(20,50)
        DO 20 I=1,ICOUNT
         IF(I.EQ.1) THEN
         IC=1
         X=ACOF(I,36)
         ELSE
         IC=ICOLD-INT((WMAXOLD-ACOF(I,36))/DXOLD)
         X=X-(WMAXOLD-ACOF(I,36))
         ENDIF
         WRITE(3,*) 'ACOF(I,36)=',ACOF(I,36),'ACOF(I,37)=',ACOF(I,37)
         WRITE(3,*) 'IC,X,WMAXOLD,ICOLD,DXOLD=',IC,X,WMAXOLD,ICOLD,
     1               DXOLD
        DO 30 II=1,1024
         WAV(IC)=X
         SP(IC)=MAX(SP(IC),SPEC(I,II))
         X=X+ACOF(I,37)
         IC=IC+1
 30     CONTINUE
         WMAXOLD=X-ACOF(I,37)
         ICOLD=IC-1
         DXOLD=ACOF(I,37)
 20     CONTINUE
         IIMAX=ICOLD
        END
        SUBROUTINE WEIGHT(WMIN,WMAX)
C
C     THIS ROUTINE WEIGHTS THE SPECTRAL COUNTS WITH THE INVERSE OF
C     THE CMA SENSITIVITY.  IT ALSO NORMALIZES THE EXPERIMENTAL SPECTRA
C     AND LOADS THE FINAL PLOTTING ARRAYS.
C
      COMMON/EXPDAT/IFDATA,WAVE(20,1030),SPEC(20,1030),WAV(20000),
     1 SP(20000),WW(20000),SPW(20000),WDAT(20),SEN(20),ICOUNT,IIMAX,
     2 INMAX,BKGRND,SLOPE
      DATA WDAT / 250.,260.,270.,280.,290.,300.,320.,350.,370.,400.,
     1            450.,500.,550.,600.,650.,700.,750.,800.,900.,1000/
C     DATA SEN /  2.89,3.16,3.32,4.26,5.22,4.2,5.53,5.55,5.04,6.1,
C    1            8.24,11.73,17.81,29.7,49.7,57.03,117.,237.,513.7,
C    1            787.97/
      DATA SEN /  .529,.576,.6,.634,.672,.755,.956,1.06,.972,1.00,
     1            1.35,1.94,2.99,4.93,8.0,9.5,19.34,37.93,1038,1669/
C
      WWMIN=WMIN/10.
      WWMAX=WMAX/10.
      II=0
      SPWMAX=1E-20
      WRITE(3,*) 'IIMAX=',IIMAX
      DO 100 I=1,IIMAX
C     WRITE(3,*) 'WWMIN,WWMAX,WAV=',WWMIN,WWMAX,WAV(I)
      IF(WAV(I).LT.WWMIN.OR.WAV(I).GT.WWMAX) GOTO 110
      J=0
      II=II+1
      IF(WAV(I).LT.WDAT(1)) THEN
```

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```
        WT=SEN(1)
      ELSE IF(WAV(I).LT.WDAT(2)) THEN
        J=2
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(3)) THEN
        J=3
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(4)) THEN
        J=4
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(5)) THEN
        J=5
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(6)) THEN
        J=6
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(7)) THEN
        J=7
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(8)) THEN
        J=8
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(9)) THEN
        J=9
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(10)) THEN
        J=10
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(11)) THEN
        J=11
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(12)) THEN
        J=12
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(13)) THEN
        J=13
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(14)) THEN
        J=14
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(15)) THEN
        J=15
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
     1      (WDAT(J)-WDAT(J-1))
      ELSE IF(WAV(I).LT.WDAT(16)) THEN
        J=16
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
```

```
      1     (WDAT(J)-WDAT(J-1))
       ELSE IF(WAV(I).LT.WDAT(17)) THEN
        J=17
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
      1     (WDAT(J)-WDAT(J-1))
       ELSE IF(WAV(I).LT.WDAT(18)) THEN
        J=18
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
      1     (WDAT(J)-WDAT(J-1))
       ELSE IF(WAV(I).LT.WDAT(19)) THEN
        J=19
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
      1     (WDAT(J)-WDAT(J-1))
       ELSE IF(WAV(I).LT.WDAT(20)) THEN
        J=20
        WT=SEN(J-1)+(WAV(I)-WDAT(J-1))*(SEN(J)-SEN(J-1))/
      1     (WDAT(J)-WDAT(J-1))
       ELSE IF(WAV(I).GT.WDAT(20)) THEN
        WT=SEN(20)
        ENDIF
C SHIFT EXP. SPECTRA TO LEFT BY 6 ANGSTROMS DUE EXP. CAL. ERROR
        WW(II)=WAV(I)*10.-6
        SPW(II)=SP(I)*WT-(BKGRND+SLOPE*(WW(II)-WMIN))
C        SPW(II)=SP(I)*WT
C    ELLIMINATE NH PEAK FROM DATA NORMALIZATION--OR OTHER PEAKS IF
C    SO DESIRED.
        IF(3345.LT.WW(II).AND.3375.GT.WW(II)
      1 .OR.5250.LT.WW(II).AND.5340.GT.WW(II)) THEN
C   DO NOTHING
        ELSE
        SPWMAX=MAX(SPW(II),SPWMAX)
        ENDIF
  110   CONTINUE
  100   CONTINUE
        INMAX=II
        WRITE(3,*) 'INMAX=',INMAX
C    NORMALIZE THE EXPERIMENTAL SPECTRA TO THE HIGHEST NON-
C    EXCLUDED PEAK
        DO 200 I=1,INMAX
        SPW(I)=SPW(I)/SPWMAX
C        WRITE(3,*) 'WW,SPW=',WW(I),SPW(I)
  200   CONTINUE
C    CHOP OFF UNWANTED LINES EXTENDING OUTSIDE OF THE PLOTTING
C    AREA
        DO 210 I=1,INMAX
        IF(SPW(I).GT.1.01)SPW(I)=1.
  210   CONTINUE
        RETURN
        END
```

```
  2   7   1C   2
.C028 .0193 .0637 .1315 .1908 .2C65 .1727 .1142 .C605 .0259
.0137 .0658 .1329 .1365 .0608 .0C13 .0344 .1171 .1606 .1375
.C357 .1121 .1178 .C3C3 .C072 .0781 .0896 .C212 .C076 .0817
.C656 .1238 .C458 .0C48 .0738 .C557 4.E-5 .0511 .0849 .0245
.C952 .0951 .0015 .0537 .0562 3.E-5 .0554 .0523 3.E-5 .0513
.1164 .0484 .C143 .0695 .0043 .0412 .C467 .0CC6 .0564 .0383
.1249 .0119 .C496 .0343 .0136 .0553 .C005 .0466 .C297 .0C76
.C031 .0211 .C679 .1369 .1944 .2C61 .1691 .1C96 .C57C .0239
.C153 .0707 .1373 .1342 .0546 .0CC3 .0407 .1235 .1612 .1333
.C395 .1176 .1151 .0246 .0111 .0837 .0855 .C159 .0119 .09C2
.C717 .1253 .C392 .0C84 .0784 .0493 .C003 .0585 .C82C .0191
.1027 .0908 .C002 .C6C5 .C501 .0C11 .C614 .0456 .C0C5 .0590
.1236 .0413 .C208 .0679 .0014 .0484 .C4CC .0C31 .C613 .03C4
.130C .0C72 .0573 .C270 .0206 .0517 9.E-5 .0522 .C219 .0140
```

Franck-Condon Factors (File: FRANK.CON)

```
1.5951 1.6164 1.6383 1.6607 1.6837 1.7074 1.7320 1.7410 1.741C 1.741C
1.5811 1.6019 1.6230 1.6444 1.6656 1.6716 1.7186 1.7410 1.741C 1.741C
1.5676 1.5877 1.6080 1.6273 1.6588 1.6758 1.6972 1.7169 1.741C 1.741C
1.5544 1.5740 1.5930 1.6229 1.6379 1.6575 1.5644 1.7C78 1.729C 1.741C
1.5417 1.5606 1.5699 1.6C30 1.6216 1.7599 1.6679 1.6872 1.5298 1.7398
1.5293 1.5472 1.5715 1.5882 1.60C5 1.6318 1.6498 1.7C60 1.6977 1.7164
1.5172 1.5331 1.5567 1.5736 1.5997 1.6155 1.6C72 1.66C1 1.6771 1.7139
1.5886 1.61C2 1.6322 1.6548 1.678C 1.7018 1.7265 1.741C 1.741C 1.741C
1.5744 1.5955 1.6168 1.6384 1.6556 1.646C 1.7126 1.7357 1.741C 1.741C
1.56C6 1.5812 1.6C17 1.6209 1.6513 1.6698 1.6914 1.71C3 1.741C 1.741C
1.5472 1.5672 1.5864 1.6145 1.6316 1.6513 1.7186 1.7C17 1.7231 1.741C
1.5342 1.5536 1.5473 1.5963 1.6151 1.6579 1.6616 1.68C9 1.7485 1.7336
1.5215 1.540C 1.5636 1.5814 1.5881 1.6251 1.6432 1.6818 1.6913 1.7097
1.5091 1.5252 1.5492 1.5665 1.5918 1.6088 1.7C29 1.6534 1.67CC 1.7048
```

R-centroids (File: RCENTROID.DAT)

```
        4              3
       0.          .769602
   1218.7     -.0063
     -7.28     0.
  30294.9      .5562
     797.31  -.0C48
     -3.72     0.
    221.5       .775156
   1218.70    -.0C63
     -7.28     0.
  3C384.1      .6C13
     798.78  -.0C46
     -3.59  0.
```

Dunham Coefficients (File: DUNHAM.COF)

```
7
.313 .110 .1CC .C6 .C424 .0000625 .0CC003
.188 .066 .06C .C360 .0254 .CC003750€ .0C0002
```

Vibrational Population Weights (File: POPLTN.WT)

```
          F30030
           32030
           34030
           36030
           38030
           40030
           42030
           44030
           46030
           48030
           5C030
           52030
```

List of Experimental OMA Files (File: FILE.OMA)

```
40C0.000              420C.00C            1.C0CC0C          12CC.CC0           45C.00C0
S(B->X) SPECTRUM AT 3 TORR                          0.00CC00CE+0C   0.C00CC00E+C0
          0               1     20C.00CC
1.00C0C0
        1                       1
```

Input File Generated by Code (File: INPUT.DAT)
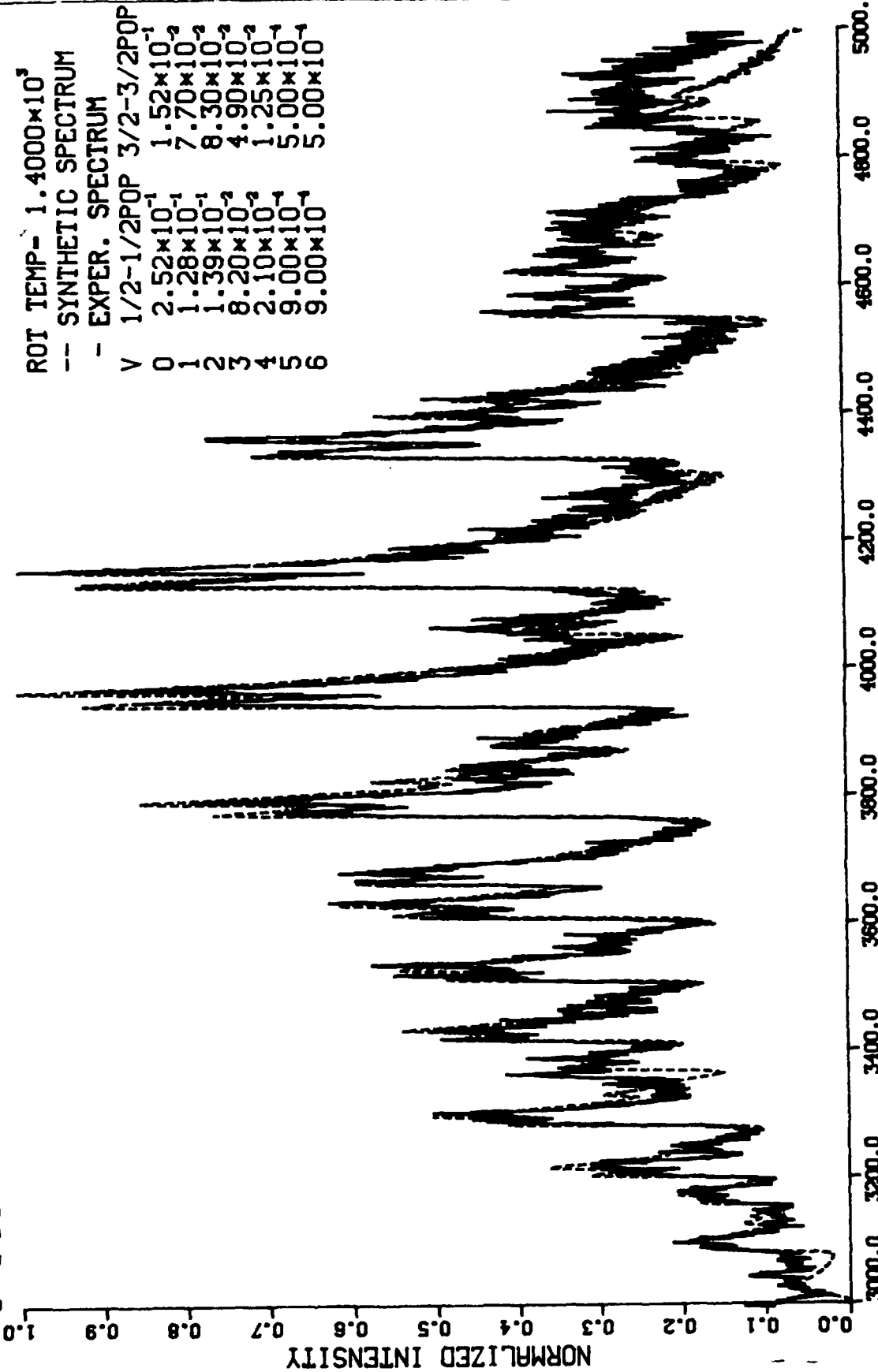
NS(B) SPECTRUM AT .74 TORR

FIGURE 2

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3. M. Born and R. Oppenheimer, Ann Physik 84, 457 (1927).

4. Condon and Shortly, The Theory of Atomic Spectra (Cambridge Univ. Press, 1935).

5. Obase, et. al., J. Chem Phys 89, 257 (1988).

6. K.P. Huber and G. Herzberg, Molecular Spectra and Molecular Structure, Vol. IV., VNR C1979, p 486–487.